FILE 'HOME' ENTERED AT 13:37:20 ON 11 MAR 2003

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 13:37:30 ON 11 MAR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7 DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

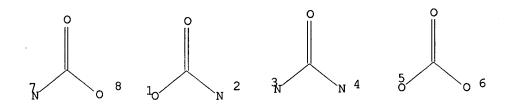
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10025947 rce first action.str

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



G1 CH2,O,S,N,[@1-@2],[@3-@4],[@5-@6],[@7-@8] G2 O,S

Structure attributes must be viewed using STN Express query preparation.

16 ANSWERS

=> search 11 sss sam
SAMPLE SEARCH INITIATED 13:38:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 561163 TO ITERATE

0.2% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000 PROJECTED ANSWERS: EXCEEDS 173898

L2 16 SEA SSS SAM L1

=> d scan

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Heptanoic acid, 7-[[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-oxo-1-cyclopenten-1-yl]thio]-, methyl ester, (R)- (9CI)

MF C19 H34 O4 S Si

Absolute stereochemistry.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):16

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN L-Glutamine,

N-acetyl-L-.alpha.-aspartyl-L-phenylalanyl-L-.alpha.-glutamyl-

L-.alpha.-aspartyl-L-isoleucyl-L-prolyl-L-lysyl-L-.alpha.-glutamyl-L-

tyrosyl-L-leucyl-, cyclic (4.fwdarw.7)-peptide (9CI)

SQL 11

MF C66 H93 N13 O22

Absolute stereochemistry.

PAGE 1-A

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Nonanoic acid, 9-[[3-O-benzoyl-4,6-O-(phenylmethylene)-.beta.-D-glucopyranosyl]oxy]-, methyl ester, (R)- (9CI) C30 H38 O9 IN

MF

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2003 ACS L2 16 ANSWERS

Decanoic acid, 10-oxo-10-[(4-phosphonophenyl)amino]- (9CI) IN

C16 H24 N O6 P MF

REGISTRY COPYRIGHT 2003 ACS L216 ANSWERS

1(2H)-Pyrimidinepropanesulfonic acid, 5-[[7-(diethylamino)-2-(1,1-IN dimethylethyl)-4H-1-benzopyran-4-ylidene]ethylidene]-3-[6-[(2,5-dioxo-1pyrrolidinyl)oxy]-6-oxohexyl]tetrahydro-2,4,6-trioxo-, sodium salt (9CI) C36 H46 N4 O11 S . Na MF

● Na

16 ANSWERS REGISTRY COPYRIGHT 2003 ACS L2 5-Heptenoic acid, 7-[2-(4-morpholinyl)-5-(1-naphthalenylmethoxy)-3-

oxocyclopentyl]-, methyl ester, [1.alpha.(Z),2.beta.,5.alpha.]- (9CI)

MF C28 H35 N O5

Relative stereochemistry. Double bond geometry as shown.

MeO (CH2)
$$\frac{1}{3}$$
 $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

CM 1

Absolute stereochemistry.

CM 2

$$\begin{array}{c} ^{\rm NH_2} \\ | \\ {\rm HO-CH_2-C-CH_2-OH} \\ | \\ {\rm CH_2-OH} \end{array}$$

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN L-Cysteinamide,

D-phenylalanyl-L-cysteinyl-L-tyrosyl-L-tryptophyl-N6-[(9H-

fluoren-9-ylmethoxy)carbonyl]-L-lysyl-L-threonyl-N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)propyl]-, cyclic (2.fwdarw.7)-disulfide (9CI)

SQL 8

MF C64 H76 N10 O13 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 2-B

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Glycine, L-threonyl-L-.alpha.-aspartyl-L-isoleucyl-L-.alpha.-aspartyl-L-

.alpha.-glutamyl-L-cysteinyl-L-.alpha.-glutamyl-L-asparaginylglycylglycyl-

L-phenylalanyl-L-cysteinyl-L-serylglycyl-L-valyl-L-cysteinyl-L-histidyl-L-asparaginyl-L-leucyl-L-prolylglycyl-L-threonyl-L-phenylalanyl-L-alpha.-glutamyl-L-cysteinyl-L-isoleucyl-L-seryl-, cyclic (6.fwdarw.12), (16.fwdarw.25)-bis(disulfide) (9CI)

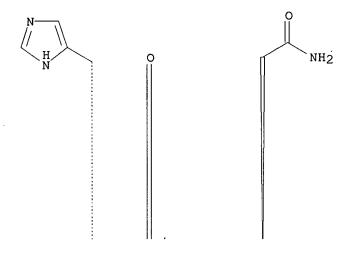
SQL 28

MF C119 H174 N32 O45 S4

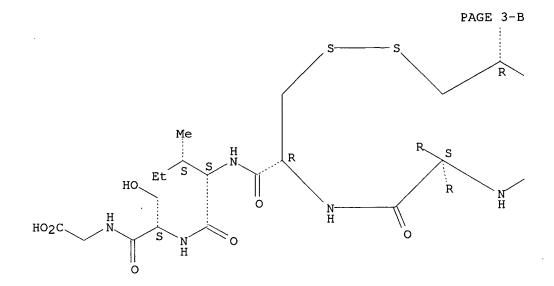
RELATED SEQUENCES AVAILABLE WITH SEQLINK

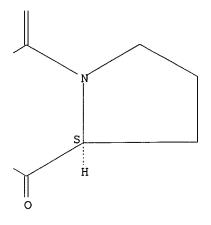
Absolute stereochemistry.

PAGE 1-B



PAGE 2-D





PAGE 4-A



L2

16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
Propanedioic acid, 1,3-phenylenebis(methylene) bis[[3,5-bis[[12-(1,1-dimethylethoxy)-12-oxododecyl]oxy]phenyl]methyl] ester (9CI)
C92 H146 O20 IN

MF

PAGE 1-A

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Prosta-5,13-dien-1-oic acid, 11,15-dihydroxy-12-methyl-9-oxo-, (5Z,11.alpha.,13E,15S)-(.+-.)- (9CI)

MF C21 H34 O5

Relative stereochemistry.
Double bond geometry as shown.

O
$$\mathbb{Z}$$
 $(CH_2)_3$ CO_2H

R \mathbb{R} \mathbb{E} \mathbb{S} $(CH_2)_4$

Me

OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 5-Heptenoic acid, 7-[3-(phenoxymethyl)-7-oxabicyclo[2.2.1]hept-2-yl]-,
 methyl ester, [1R-[1.alpha.,2.alpha.(Z),3.alpha.,4.alpha.]]- (9CI)

MF C21 H28 O4

Absolute stereochemistry.

Double bond geometry as shown.

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Dodecanoic acid, 12-[[3-(3-carboxypropoxy)-2-pyridinyl]amino]-12-oxo-(9CI)

MF C21 H32 N2 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN L-Glutamine, N2-[(1,1-dimethylethoxy)carbonyl]-N-(4-hydroxyphenyl)-,
 methyl ester (9CI)

MF C17 H24 N2 O6

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Hexanoic acid, 6-[2-[1-[4-(dimethylamino)-4-oxo-3,3-diphenylbutyl]-4-hydroxy-4-piperidinyl]phenoxy]-, ethyl ester, monohydrochloride (9CI)

MF C37 H48 N2 O5 . Cl H

● HCl

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 3-Cyclopentene-1-heptanoic acid, 2-oxo-, methyl ester (9CI)

MF C13 H20 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

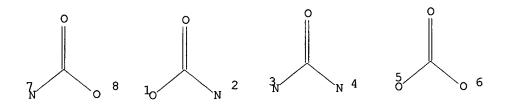
=>
Uploading 10025947 rce first action.str

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR



G1 CH2,O,S,N,[@1-@2],[@3-@4],[@5-@6],[@7-@8] G2 O, S

Structure attributes must be viewed using STN Express query preparation.

7 ANSWERS

=> search 13 sss sam SAMPLE SEARCH INITIATED 13:43:04 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 561163 TO ITERATE

0.2% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

INCOMPLETE FULL FILE PROJECTIONS: ONLINE

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000 PROJECTED ANSWERS: **EXCEEDS** 74805

L47 SEA SSS SAM L3

=> d scan

L4

7 ANSWERS REGISTRY COPYRIGHT 2003 ACS Propanedioic acid, 1,3-phenylenebis(methylene) bis[[3,5-bis[[12-(1,1-IN dimethylethoxy)-12-oxododecyl]oxy]phenyl]methyl] ester (9CI)

MF C92 H146 O20

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Nonanoic acid, 9-[[3-0-benzoyl-4,6-0-(phenylmethylene)-.beta.-Dglucopyranosyl]oxy]-, methyl ester, (R)- (9CI)

MF C30 H38 O9

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Heptanoic acid, 7-[[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-oxo-1-cyclopenten-1-yl]thio]-, methyl ester, (R)- (9CI)

MF C19 H34 O4 S Si

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1(2H)-Pyrimidinepropanesulfonic acid, 5-[[7-(diethylamino)-2-(1,1-dimethylethyl)-4H-1-benzopyran-4-ylidene]ethylidene]-3-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]tetrahydro-2,4,6-trioxo-, sodium salt (9CI) MF C36 H46 N4 O11 S . Na

Na

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS

$$\begin{array}{c|c} & \circ \\ & \vdash \\ & \bullet \\ & \bullet$$

HCl

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN L-Cysteinamide,
D-phenylalanyl-L-cysteinyl-L-tyrosyl-L-tryptophyl-N6-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-lysyl-L-threonyl-N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)propyl]-, cyclic (2.fwdarw.7)-disulfide (9CI)
SQL 8

RELATED SEQUENCES AVAILABLE WITH SEQLINK

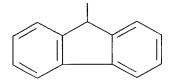
Absolute stereochemistry.

MF

C64 H76 N10 O13 S2

PAGE 1-B

1424 ANSWERS



L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 3-Cyclopentene-1-heptanoic acid, 2-oxo-, methyl ester (9CI)

MF C13 H20 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search 13 sss full FULL SEARCH INITIATED 13:45:17 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 3.2% PROCESSED 363804 ITERATIONS

< 3.4% PROCESSED 382188 ITERATIONS 1433 ANSWERS</pre>

< 3.6% PROCESSED 400000 ITERATIONS 1449 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)</pre>

SEARCH TIME: 00.02.08

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 40067

L5 1449 SEA SSS FUL L3

=> d scan

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN INDEX NAME NOT YET ASSIGNED MF C30 H36 N3 O12 P S2 . 2 K

●2 K

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 3H-Indolium,

2-[5-[1,3-dihydro-3,3-dimethyl-5-phosphono-1-(3-sulfopropyl)-

2H-indol-2-ylidene]-1,3-pentadienyl]-1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-3,3-dimethyl-5-phosphono-, inner salt, dipotassium salt (9CI) MF C38 H47 N3 O13 P2 S . 2 K

●2 K

- L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
- IN 1-Pyrrolidineheptanoic acid, 5-[(1E)-3-hydroxy-3-[5-(trifluoromethyl)-2furanyl]-1-propenyl]-3,3-dimethyl-2-oxo-, (5R)- (9CI)
- MF C21 H28 F3 N O5

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Valine, N5-[bis[[(1,1-dimethylethoxy)carbonyl]amino]methylene]-N2-[4-[3[[(1,1-dimethylethoxy)carbonyl]amino]propoxy]-3-[3-(1-methylethenyl)-4quinolinyl]benzoyl]-L-ornithyl-3-hydroxy-3-methylprolyl-2,3-didehydro(9CI)

MF C55 H76 N8 O13

Absolute stereochemistry.

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1,2,4,5-Benzenetetracarboxylic acid, polymer with (1methylethylidene)bis[4,1-cyclohexanediyloxy(2-hydroxy-3,1-propanediyl)]
di-2-propenoate, (1-methylethylidene)bis[4,1-phenyleneoxy(2-hydroxy-3,1propanediyl)] bis(2,5-dihydro-2,5-dioxo-1H-pyrrole-1-hexanoate) and
.beta.,.beta.,.beta.',.beta.'-tetramethyl-2,4,8,10tetraoxaspiro[5.5]undecane-3,9-diethanol (9CI)

MF (C41 H50 N2 O12 . C27 H44 O8 . C15 H28 O6 . C10 H6 O8)x CI PMS

CM 1

PAGE 1-A

PAGE 1-B

CM 2

PAGE 1-A

PAGE 1-B

CM 3

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{Me} \\ \text{IO-CH}_2\text{-C} & \text{O} & \text{C-CH}_2\text{-OH} \\ \text{Me} & \text{Me} & \text{Me} \end{array}$$

CM 4

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid,
6-[[2-(4-methoxyphenyl)-1-(3-methoxypropyl)-1H-benzimidazol6-yl]oxy]-, methyl ester (9CI)
MF C25 H32 N2 O5

MeO-C- (CH₂) 5-0

OMe

$$(CH_2)$$
 3-OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS IN Pentanoic acid, 5-[4-(methylthio)phenoxy]- (9CI) MF C12 H16 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Octanoic acid, 8-[4-[[[2,5-dihydro-4-hydroxy-2-oxo-1-[4-

(trifluoromethyl)phenyl]-1H-pyrrol-3-yl]carbonyl]amino]phenoxy]- (9CI)

MF C26 H27 F3 N2 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 10(9H)-Acridinehexanoic acid, 2-amino-9-oxo- (9CI)

MF C19 H20 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS IN 2H-Pyran-4-carboxylic acid, 4-[[4-(4-carboxybutoxy)phenyl]sulfonyl]tetrahy

dro-, 4-(1,1-dimethylethyl) ester (9CI) MF C21 H30 O8 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Cyclopropaneoctanoic acid, 2-hexyl-, (1R,2R)-rel- (9CI)

MF C17 H32 O2

Relative stereochemistry.

Me
$$(CH_2)$$
 5 S (CH_2) 7 CO_2H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid, 5-[2-(3-cyanopropoxy)-5-[(5,6-diethoxy-7-fluoro-1,3-dihydro-1-imino-2H-isoindol-2-yl)acetyl]-3-(1,1-dimethylethyl)phenoxy]-, monohydrobromide (9CI)

MF C33 H42 F N3 O7 . Br H

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid,

5-[2-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-dihydro-1-imino-5,6-dimethoxy-2H-isoindol-2-yl)acetyl]phenoxy]-, mono(trifluoroacetate) (9CI)

MF C27 H33 F N2 O6 . C2 H F3 O2

CM 1

$$\begin{array}{c|c} & \text{t-Bu} \\ & \text{O- (CH}_2)_4 - \text{CO}_2\text{H} \\ & \text{MeO} \end{array}$$

CM 2

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

MF C24 H28 N2 O2 . Cl H

● HCl

· L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Neodecanoic acid, oxiranylmethyl ester, polymer with butyl 2-methyl-2-propenoate, butyl 2-propenoate, .alpha.-[dimethyl[3-[(1-oxo-2-

propenyl)oxy]propyl]silyl]-.omega.-[(trimethylsilyl)oxy]poly[oxy(dimethyls ilylene)], ethenylbenzene, 2-ethylhexyl 2-propenoate, 2-hydroxyethyl 2-methyl-2-propenoate, methyl 2-methyl-2-propenoate, 2-methylpropyl 2-methyl-2-propenoate, 2-propenoic acid and 1,3,5-tris[6-[[[(1-methylpropylidene)amino]oxy]carbonyl]amino]hexyl]-1,3,5-triazine-2,4,6(1H,3H,5H)-trione (9CI)

MF (C36 H63 N9 O9 . C13 H24 O3 . C11 H20 O2 . C8 H14 O2 . C8 H14 O2 . C8 H8

C7 H12 O2 . C6 H10 O3 . C5 H8 O2 . C3 H4 O2 . (C2 H6 O Si) \rlap{n} C11 H24 O3 Si2) x

CI PMS

CM 1

CM 2

CM 3

CM 4

$$^{\rm H_2C}$$
 O $^{\rm H_2}$ $^{\rm H_2}$ $^{\rm H_2}$ $^{\rm H_2}$ $^{\rm H_2}$ $^{\rm H_2}$ $^{\rm H_2}$ OH

$$\begin{array}{c}
O \\
\parallel \\
n-BuO-C-CH \longrightarrow CH_2
\end{array}$$

CM 6

$$_{\text{CH}_2-\text{ O- C- CH}}^{\text{O}}$$
 $_{\text{CH}_2}^{\text{CH}_2}$ $_{\text{CH}_2}^{\text{CH}_2}$ $_{\text{Et-CH-Bu-n}}^{\text{O}}$

CM 7

$$H_2C = CH - Ph$$

CM 8

$$\begin{array}{c|c} & \text{O} & \text{CH}_2 \\ \parallel & \parallel \\ \text{n-BuO-C-C-Me} \end{array}$$

CM 9

$$\begin{array}{c} \text{O} \quad \text{CH}_2 \\ \parallel \quad \parallel \\ \text{i-BuO-C-C-Me} \end{array}$$

CM 10

CM 11

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 3-Thiazolidinehexanoic acid,
5-[(4-methoxyphenyl)methylene]-4-oxo-2-thioxo, 5-methyl-2-(methylthio)-4-pyrimidinyl ester (9CI)
MF C23 H25 N3 O4 S3

PAGE 1-A

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 3H-Pyrrolo[2,3-b]pyridinium, 2-[3-[1,3-dihydro-3,3-dimethyl-1-(3-

sulfopropyl)-2H-pyrrolo[2,3-b]pyridin-2-ylidene]-1-propenyl]-7-(6-ethoxy-6oxohexyl)-3,3-dimethyl-5-phosphono-, inner salt (9CI)

MF C32 H43 N4 O8 P S

CI COM

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C35 H53 N O8 Si2

Absolute stereochemistry.

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C63 H70 O6 S2

$$H_2C = CH - CH_2 O$$
 $H_2C = CH - CH_2 - CH - O - C - (CH_2)_4 - O$
 $N - Pr Pr - n$
 S

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Hexanoic acid, 6-[(2-chloro-1-phenyl-1H-benzimidazol-6-yl)oxy]-, methyl ester (9CI)

MF C20 H21 C1 N2 O3

$$\begin{array}{c|c} O & Ph \\ \parallel & \parallel \\ MeO-C-(CH_2)5-O & \parallel & \parallel \\ N & N \end{array}$$

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1H-Benzimidazole-1-propanoic acid, 6-[(6-methoxy-6-oxohexyl)oxy]-2-(4-methoxyphenyl)- (9CI)

MF C24 H28 N2 O6

MeO-C- (CH₂)₅-0

$$N$$
 N
 N
 $CH_2-CH_2-CO_2H$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

MF C78 H86 N8 O4 S16 Si

CI CCS

PAGE 2-A

PAGE 3-A

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Oxirane, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-,
homopolymer, 6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexanoate
[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]carbamate, homopolymer (9CI)

MF ((C21 H24 O4)x . x C10 H13 N O4 . x C7 H11 N O4)x

CI PMS

CM 1

CM 2

$$\begin{array}{c|c} & \text{O} & \text{CH}_2 \\ & || & || \\ & \text{HO}_2\text{C} - \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{O} - \text{C} - \text{C} - \text{Me} \end{array}$$

CM 3

CM 4

CM 5

REGISTRY COPYRIGHT 2003 ACS L5 1449 ANSWERS

Quino[2,3-b]acridine-5,12-dihexanoic acid, 7,14-dihydro-2,9-dinitro-7,14-IN dioxo-, diethyl ester (9CI) C36 H38 N4 O10

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5

1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS Carbamic acid, [3-[[1-[[[4-(acetylamino)phenyl]sulfonyl]amino]-5,6-IN dimethyl-3-oxo-3H-imidazo[5,1-c][1,4]thiazin-8-yl]thio]propyl]-, 1,1-dimethylethyl ester (9CI)

MF C24 H31 N5 O6 S3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 REGISTRY COPYRIGHT 2003 ACS 1449 ANSWERS

Benzo[1,2-c:4,5-c']dipyrrole-2,6(1H,3H)-dihexanoic acid, IN 5,7-dihydro-1,3,5,7-tetraoxo-, di-4-pentenyl ester (9CI)

MF C32 H40 N2 O8

CI COM

$$H_2C = CH - (CH_2)_3 - O - C - (CH_2)_5$$

O

O

(CH₂) 5 - C - O

PAGE 1-B

- (CH₂)₃-CH== CH₂

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid,

5-[2-(2-cyano-1,1-dimethylethyl)-4-[(5,6-diethoxy-7-fluoro-1,3-dihydro-1-imino-2H-isoindol-2-yl)acetyl]phenoxy]-, monohydrobromide (9CI)

MF C30 H36 F N3 O6 . Br H

$$\begin{array}{c|c} & \text{Me} \\ & \text{Me}-\text{C}-\text{CH}_2-\text{CN} \\ & \text{O}-\text{(CH}_2)_4-\text{CO}_2\text{H} \\ & \text{Eto} \\ & \text{Eto} \end{array}$$

• HBr

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IN Pentanoic acid, 5-[2-(3-cyanopropoxy)-6-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]phenoxy]-, monohydrobromide (9CI)

MF C33 H42 N4 O7 . Br H

HBr

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IN Carbamic acid, [7-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)heptyl]-, 4-methoxyphenyl ester (9CI)

MF C31 H35 N3 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Oxirane, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-, homopolymer, 2,5-dihydro-2,5-dioxo-1H-pyrrole-1-hexanoate (9CI)

MF (C21 H24 O4)x . x C10 H13 N O4

CI COM

CM 1

CM 2

CM 3

$$\begin{array}{c|c} O & \text{CH}_2-O & \text{Me} \\ \hline & CH_2-O & \text{Me} \\ \hline & Me \\ \end{array}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

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IN 3-Thiazolidinehexanoic acid, 5-[(2,4-dihydroxyphenyl)methylene]-4-oxo-2-thioxo- (9CI)

MF C16 H17 N O5 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN INDEX NAME NOT YET ASSIGNED

MF (C40 H65 N7 O14 . C15 H24 O6 . (C2 H4 O)n C20 H24 N2 O7)x

CI PMS

CM 1

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CM 2

CM 3

3 (D1-Me)

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IN INDEX NAME NOT YET ASSIGNED

MF C32 H40 N4 O8 S2 . K

HO3S
$$CH-CH=CH-CH=CH$$
 N N $N+$ $N+$ $CH_2)$ $3-SO_3H$ (CH_2) $5-CO_2-$

K

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IN 1-Pyrrolidineheptanoic acid, 2-[(1E,3S)-3-hydroxy-4-(2'-methoxy[1,1'-biphenyl]-3-yl)-1-butenyl]-5-oxo-, (2R)- (9CI)

MF C28 H35 N O5

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 1-Pyrrolidineheptanoic acid, 2-[(1E)-3-[1,1'-biphenyl]-2-yl-3-hydroxy-1-propenyl]-5-oxo-, (2R)- (9CI)

MF C26 H31 N O4

Absolute stereochemistry. Double bond geometry as shown.

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Hexanoic acid, 6-[[1-phenyl-2-[(phenylmethyl)sulfonyl]-1H-benzimidazol-6-IN yl]oxy]- (9CI) C26 H26 N2 O5 S

MF

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Heptanoic acid, 7-[2,3-dimethoxy-6-(1-piperazinylmethyl)phenoxy]-, IN dihydrochloride (9CI)

C20 H32 N2 O5 . 2 Cl H MF

MeO
$$CH_2$$
 NH $O-(CH_2)_6$ CO_2H

●2 HCl

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1(2H)-Pyrimidinehexanoic acid,
5-[[7-(diethylamino)-4-(1,1-dimethylethyl)2H-1-benzopyran-2-ylidene]ethylidene]tetrahydro-2,4,6-trioxo-3-(3-sulfopropyl)-, monosodium salt (9CI)
MF C32 H43 N3 O9 S . Na

Na

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Absolute stereochemistry.

Double bond geometry unknown.

MeO OH OH Bu-t
$$i-Pr S N OH OH$$

$$HO_2C (CH_2)_4$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Undecanoic acid, 11-[4-[(1E)-(4-heptylphenyl)azo]phenoxy]-, ethenyl ester,

polymer with ethenol (9CI)

MF (C32 H46 N2 O3 . C2 H4 O)x

CI PMS

CM 1

Double bond geometry as shown.

CM 2

 $H_2C = CH - OH$

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IN Pentanoic acid, 5-[4-[(5,6-diethoxy-7-fluoro-1,3-dihydro-1-imino-2H isoindol-2-yl)acetyl]-2-(1,1-dimethylethyl)-6-(2-methyl-1 pyrrolidinyl)phenoxy]-, monohydrobromide (9CI)
MF C34 H46 F N3 O6 . Br H

Eto
$$CH_2$$
 CH_2 $CH_$

• HBr

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MF C28 H35 N5 O6 . Br H

$$\begin{array}{c|c} O & NH & O & CH_2 - C & \\ \hline MeNH-C & N & CH_2-C & N & \\ \hline Eto & & & \\ \end{array}$$

• HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzaldehyde, 4-nitro-, O-[[[6-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxime (9CI)

MF C30 H31 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Hexanoic acid, 6-(9H-carbazol-2-yloxy)-, ethyl ester (9CI)

MF C20 H23 N O3

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 3-Thiazolidinehexanoic acid, 5-[(2,4-dichlorophenyl)methylene]-4-oxo-2-thioxo-, methyl ester (9CI)

MF C17 H17 C12 N O3 S2

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN INDEX NAME NOT YET ASSIGNED

MF C15 H20 Br N O3

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C34 H38 N4 O8 S

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

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Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Carbamic acid,

[4-[3-[4-[[(1,1-dimethylethoxy)carbonyl](phenylmethoxy)amin o]butyl]tetrahydro-2,4,6-trioxo-1,3,5-triazin-1(2H)-yl]butyl](phenylmethoxy)-, 2,2,2-trichloroethyl ester (9CI) MF C33 H42 C13 N5 O9

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IN 1-Piperazineheptanoic acid, 4-[[2-(3-carboxypropoxy)-3,4- dimethoxyphenyl]methyl]-, dihydrochloride (9CI)

MF C24 H38 N2 O7 . 2 Cl H

$$CH_2$$
 N $O-(CH_2)_3-CO_2H$ OMe

●2 HCl

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MF C22 H24 N2 O3

$$_{\mathrm{HO_{2}C-}}$$
 (CH₂) 5-0 $_{\mathrm{CH_{2}-CH==CH_{2}}}^{\mathrm{Ph}}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzoic acid, 4-[[6-(oxiranylmethoxy)-6-oxohexyl]oxy]-,
2-fluoro-4-[[4-[[6-[[4-[[6-(oxiranylmethoxy)-6oxohexyl]oxy]benzoyl]oxy]hexyl]oxy]phenyl]ethynyl]phenyl ester (9CI)

MF C52 H57 F O13

CI COM

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$$-(CH_2)_{6}-0-C$$

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IN. Decanoic acid,
10-[4-[[[6-[(4-chlorophenyl)methoxy]-1,2-dihydro-4-hydroxy2-oxo-3-quinolinyl]carbonyl]amino]phenoxy]- (9CI)
MF C33 H35 Cl N2 O7

C1
$$CH_2-O$$
 CH_2-O CH_2-O $O-(CH_2)_9-CO_2H$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Carbamic acid, [3-[(8-amino-1,5-naphthyridin-2-yl)oxy]propyl]-,

1,1-dimethylethyl ester (9CI) MF C16 H22 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Prostan-1-oic acid, 15-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-16,16difluoro-9-oxo-11-[(tetrahydro-2H-pyran-2-yl)oxy]-, (11.alpha.)- (9CI)
MF C31 H56 F2 O6 Si

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Pentanoic acid, 5-[4-[(2-cyclopropyl-5,7-dihydro-7-imino-6H-pyrrolo[3,4-b]pyridin-6-yl)acetyl]-2-(1,1-dimethylethyl)-6-[3-(methoxymethyl)-1-pyrrolidinyl]phenoxy]-, monohydrobromide (9CI)

MF C33 H44 N4 O5 . Br H

NH O (CH₂)
$$_4$$
 - CO₂H $_1$ CH₂ - OMe

HBr

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IN Pentanoic acid,

5-[2-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-dihydro-1-imino-

• HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Pentanoic acid, 5-[4-[(2-cyclopropyl-5,7-dihydro-7-imino-6H-pyrrolo[3,4-b]pyridin-6-yl)acetyl]-2-(1,1-dimethylethyl)-6-(1-pyrrolidinyl)phenoxy]-,
mono(trifluoroacetate) (9CI)

MF C31 H40 N4 O4 . C2 H F3 O2

CM 1

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1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris[6-[[[(1-IN methylpropylidene)amino]oxy]carbonyl]amino]hexyl]-, polymer with 3-(triethoxysily1)-1-propanamine and Udaburu S 2818 (9CI)

(C36 H63 N9 O9 . C9 H23 N O3 Si . Unspecified)x MF

CI **PMS**

> CM 1

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM

CM

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2H-Isoindole-2-hexanoic acid, 1,3-dihydro-4-nitro-1,3-dioxo-, IN 4-(2-cyano-3-methoxy-3-oxo-1-propenyl)-2-methoxyphenyl ester (9CI)

MFC26 H23 N3 O9

NC O
$$CH = C - C - OMe$$

NC O $CH = C - C - OMe$

NO OMe

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IN Oxiraneoctanoic acid, 3-[(3-pentyloxiranyl)methyl]-, 1-[[(1-

oxohexadecyl)oxy]methyl]-1,2-ethanediyl ester (9CI) MF C55 H98 O10

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 3H-Pyrrolo[2,3-b]pyridinium, 2-[3-[2,4-dihydro-5-methyl-4-phenyl-2-(3-sulfopropyl)-3H-1,2,4-triazol-3-ylidene]-1-propenyl]-7-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-3,3-dimethyl-5-phosphono-, inner salt, monopotassium salt (9CI)

MF C34 H41 N6 O10 P S . K

K

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Benzoxazolium, 2-[7-[3-(5-carboxypentyl)-5-phosphono-2(3H)-benzothiazolylidene]-1,3,5-heptatrienyl]-5-phosphono-3-(3-sulfopropyl)-, IN inner salt, dipotassium salt (9CI) C30 H34 N2 O12 P2 S2 . 2 K

MF

PAGE 1-A

2 K

PAGE 1-B

-- PO3H2

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IN 1-Pyrrolidineheptanoic acid, 2-[(1E)-3-[3-(3-fluorophenoxy)phenyl]-3hydroxy-1-propenyl]-5-oxo-, (2R)- (9CI)
MF C26 H30 F N O5

Absolute stereochemistry.

Double bond geometry as shown.

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IN Cholest-5-en-3-ol (3.beta.)-, 5-(4-ethynylphenoxy)pentanoate (9CI)

MF C40 H58 O3

Absolute stereochemistry.

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CHMe2

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L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid,
6-[[2-(4-methoxyphenyl)-1-(3-methoxypropyl)-1H-benzimidazol6-yl]oxy]- (9CI)
MF C24 H30 N2 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-Isoindole-2-octanoic acid, 1,3-dihydro-1,3-dioxo-5[(tricyclo[3.3.1.13,7]dec-1-yloxy)carbonyl]- (9CI)
MF C27 H33 N O6

1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS L5

2-Furannonanoic acid, 2,5-dihydro-, methyl ester (9CI) IN

MF C14 H24 O3

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2H-Pyrano[3,2-g]quinoline-6-methanesulfonic acid,

9-[6-[(2,5-dioxo-3-sulfo-

1-pyrrolidinyl)oxy]-6-oxohexyl]-8,9-dihydro-8,8-dimethyl-2-oxo-4-(trifluoromethyl) - (9CI)

C26 H27 F3 N2 O12 S2

MF CI COM

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid,
6-[[5,6-dimethyl-1-[[(4-methylphenyl)sulfonyl]amino]-3-oxo3H-imidazo[5,1-c][1,4]thiazin-8-yl]thio]-, ethyl ester (9CI)
MF C23 H29 N3 O5 S3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Tetradecanoic acid,

(2R)-2-[[6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-1oxohexyl]oxy]-3-(phosphonooxy)propyl ester, monoammonium salt (9CI)

MF C29 H47 N4 O11 P . H3 N

Absolute stereochemistry.

Me (CH₂)
$$\frac{1}{12}$$
 O R O (CH₂) $\frac{1}{5}$ NH O NO2

• инз

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid,
5-[2-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]-6-(4-morpholinyl)phenoxy]-, monohydrobromide (9CI)
MF C33 H44 N4 O7 . Br H

MeNH-C
$$CH_2$$
-C CH_2) $4-CO_2H$

• HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid,
5-[2-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-dihydro-1-imino
5,6-dimethoxy-2H-isoindol-2-yl)acetyl]-6-(3-fluoro-1-pyrrolidinyl)phenoxy], methyl ester, monohydrochloride (9CI)
MF C32 H41 F2 N3 O6 . C1 H

HCl

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

MF C29 H29 F2 N3 O2

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L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Carbamic acid,

MF C45 H53 C1 N8 O5

Relative stereochemistry.

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IN 3-Thiazolidineundecanoic acid, 5-[[4-(dimethylamino)phenyl]methylene]-4-oxo-2-thioxo-(9CI)

MF C23 H32 N2 O3 S2

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IN Hexanoic acid, 6-[(O-.alpha.-D-mannopyranosyl-(1.fwdarw.3)-O-[.alpha.-D-

mannopyranosyl-(1.fwdarw.6)]-.alpha.-D-mannopyranosyl)oxy]-, methyl ester
(9CI)

MF C25 H44 O18

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 3H-Pyrrolo[2,3-b]pyridinium, 7-(5-carboxypentyl)-2-[3-[1,3-dihydro-3,3-

MF C31 H40 N4 O5 S2

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1-Pyrrolidineheptanoic acid, 2-[(1E,3S)-3-hydroxy-4-(2-methylphenyl)-1-butenyl]-5-oxo-, (2R)- (9CI)

MF C22 H31 N O4

Absolute stereochemistry.
Double bond geometry as shown.

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IN 1-Pyrrolidineheptanoic acid, 2-[(1E)-3-hydroxy-3-(3-hydroxyphenyl)-1-propenyl]-5-oxo-, (2R)- (9CI)

MF C20 H27 N O5

Absolute stereochemistry. Double bond geometry as shown.

$$CO_2H$$
OH
 R
 E
OH
OH

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MF C25 H25 N3 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Hexanoic acid, 6-[[2-(4-methoxyphenyl)-1-[3-[methyl(2-methyl-1-oxopropyl)amino]propyl]-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI)

MF C29 H39 N3 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid,
6-[[1-(cyclohexylmethyl)-2-phenyl-1H-benzimidazol-5-yl]oxy], methyl ester (9CI)
MF C27 H34 N2 O3

$$\begin{array}{c} O \\ \parallel \\ MeO-C-(CH_2)_5-O \\ \hline \\ N \\ \hline \\ N-CH_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid,
5-[[3-(hexyloxy)-4-hydroxy-2-oxo-2H-1-benzopyran-5-y1]oxy], ethyl ester (9CI)
MF C22 H30 O7

$$\begin{array}{c|c}
0 & O \\
0 & O \\
\hline
\text{CH}_2)_5 - \text{Me}
\end{array}$$
EtO-C-(CH₂)₄-O OH

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Pentanoic acid, 5,5',5''-[(2,4,6-trioxo-1,3,5-triazine-1,3,5(2H,4H,6H)triyl)tris(6,1-hexanediyliminocarbonyloxy)]tris-, tris[2-[(1-oxo-2propenyl)oxy]ethyl] ester (9CI)

MF C54 H84 N6 O21

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H₂C=CH-C-O-CH₂-CH₂-O-C-(CH₂)₄-O-C-NH-(CH₂)₆

H₂C=CH-C-O-CH₂-CH₂-O-C-(CH₂)₄-O-C-NH-(CH₂)₆

PAGE 1-B

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MF C20 H20 F3 N3 O5 S3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
=> save temp 15 gencmpds/a
ANSWER SET L5 HAS BEEN SAVED AS 'GENCMPDS/A'
=> e Hexanoic acid, 6-[[1-phenyl-2-(phenylamino)-1H-benzimidazol-6-yl]oxy]-/cn
                   HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER,
E1
S-OXI
                   DE, (ENDO, ANTI) -/CN
E2
                   HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER,
S-OXI
                   DE, (EXO, ANTI) -/CN
             0 --> HEXANOIC ACID, 6-1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-
E3
                   6-YL OXY-/CN
                   HEXANOIC ACID,
             1
E4
6-(((((((((3,4-DICHLOROPHENYL)METHYL)AMINO)IMIN
                   OMETHYL) AMINO) IMINOMETHYL) AMINO) -/CN
                   HEXANOIC ACID,
             1
6-((((((17.ALPHA.)-17-HYDROXYPREGN-4-EN-20-YN
                    -3-YLIDENE) AMINO) OXY) ACETYL) AMINO) -/CN
                   HEXANOIC ACID,
6-((((((2-(((3,5-BIS(1,1-DIMETHYLETHYL)-2-HYD
ROXYPHENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) P
                   HENYLACETYL) AMINO) -, (1R-(1.ALPHA.(S*), 2.BETA.)) -/CN
             1
                   HEXANOIC ACID,
6-((((((2-(((3,5-DIBROMO-2-HYDROXYPHENYL)METH
YLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) PHENYLACETYL) AMI
                   NO)-, (1R-(1.ALPHA.(S*),2.BETA.))-/CN
                   HEXANOIC ACID,
E.R
             1
6-((((((2-(((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-
5-METHOXYPHENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AM
                   INO) PHENYLACETYL) AMINO) -, (1R-(1.ALPHA.(S*), 2.BETA.)) -/CN
                   HEXANOIC ACID,
6-((((((2-(((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-
5-NITROPHENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMIN
                   O) PHENYLACETYL) AMINO) -, (1R-(1.ALPHA.(S*), 2.BETA.)) -/CN
                   HEXANOIC ACID,
6-((((((2-(((3-(1,1-DIMETHYLETHYL)-2-HYDROXYP
HENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) PHENYL
                   ACETYL)AMINO) -, (1R-(1.ALPHA.(S*), 2.BETA.)) -/CN
                   HEXANOIC ACID,
E11
6-((((((2-(((5-(1,1-DIMETHYLETHYL)-2-HYDROXYP
HENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) PHENYL
                   ACETYL)AMINO) -, (1R-(1.ALPHA.(S*), 2.BETA.)) -/CN
                   HEXANOIC ACID,
6-(((((2-((2-((1-NAPHTHALENYLCARBONYL)AMINO)
```

-1-OXO-3-(1-(TRIPHENYLMETHYL)-1H-IMIDAZOL-4-YL)PROPYL)AMINO)

(1S-(1.ALPHA.,

CYCLOHEXYL) OXY) CARBONYL) AMINO) ACETYL) AMINO) -,

```
2.BETA.(R*)))-/CN
```

```
=> e Hexanoic acid, 6-((1-phenyl-2-(phenylamino)-1H-benzimidazol-6-yl)oxy)-/cn
                   HEXANOIC ACID,
             1
6-((1-PHENYL-2-(4-PYRIDINYL)-1H-BENZIMIDAZOL-
                   6-YL) OXY) -/CN
                   HEXANOIC ACID,
             1
6-((1-PHENYL-2-(4-PYRIDINYL)-1H-BENZIMIDAZOL-
                   6-YL)OXY)-, METHYL ESTER/CN
             1 --> HEXANOIC ACID,
6-((1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-
                   6-YL) OXY) -/CN
                   HEXANOIC ACID,
             1
6-((1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-
                   6-YL)OXY)-, METHYL ESTER/CN
                   HEXANOIC ACID,
             1
6-((1-PHENYL-2-(PROPYLAMINO)-1H-BENZIMIDAZOL-
                   6-YL) OXY) -/CN
             1
                   HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLAMINO)-1H-BENZIMIDAZOL-
                   6-YL)OXY)-, METHYL ESTER/CN
                   HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLSULFINYL)-1H-BENZIMIDAZ
                   OL-6-YL)OXY)-, METHYL ESTER/CN
             1
                   HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLSULFONYL)-1H-BENZIMIDAZ
                   OL-6-YL)OXY)-/CN
                   HEXANOIC ACID,
             1
6-((1-PHENYL-2-(PROPYLSULFONYL)-1H-BENZIMIDAZ
                   OL-6-YL)OXY)-, METHYL ESTER/CN
                   HEXANOIC ACID,
             1
6-((1-PHENYL-2-(PROPYLTHIO)-1H-BENZIMIDAZOL-6
                   -YL)OXY)-/CN
                   HEXANOIC ACID,
E11
             1
6-((1-PHENYL-2-(PROPYLTHIO)-1H-BENZIMIDAZOL-6
                   -YL)OXY)-, METHYL ESTER/CN
                   HEXANOIC ACID, 6-((1-PHENYLETHYL)AMINO)-, ETHYL ESTER/CN
E12
=> e3
             1 "HEXANOIC ACID,
L6
6-((1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-6-Y
               L) OXY) -"/CN
=> d 16
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
1.6
     488141-30-6 REGISTRY
RN
CN
     Hexanoic acid, 6-[[1-phenyl-2-(phenylamino)-1H-benzimidazol-6-yl]oxy]-
            (CA INDEX NAME)
      (9CI)
FS
     3D CONCORD
     C25 H25 N3 O3
MF
SR
     STN Files: CA, CAPLUS
LC
```

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 165.25 165.46

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 13:55:02 ON 11 MAR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11 FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 16

L7 1 L6

=> d 17 ti fbib abs

- L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
- TI Preparation of benzimidazoles for treatment of microglia-activation associated diseases
- AN 2003:58064 CAPLUS
- DN 138:106701
- TI Preparation of benzimidazoles for treatment of microglia-activation associated diseases
- IN Blume, Thorsten; Halfbrodt, Wolfgang; Kuhnke, Joachim; Moenning, Ursula; Schneider, Herbert

```
Schering Aktiengesellschaft, Germany
PA
     PCT Int. Appl., 96 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     German
LΑ
FAN.CNT 1
                      KIND
                            DATE
                                           APPLICATION NO.
                                                            DATE
     PATENT NO.
                                           _____
     -------
                            20030123
                                           WO 2002-EP7561
                                                            20020705
     WO 2003006438
PΙ
                       Α1
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM,
             HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
                                           DE 2001-10135050A 20010709
                                           DE 2001-10135050 20010709
     DE 10135050
                       A1
                            20030206
os
     MARPAT 138:106701
GI
```

AB The title compds. [I; R1 = (substituted) aryl, 5-6 membered heteroaryl; Z = NH, NR4, O, S, SO, SO2; R2, R4 = perfluoroalkyl, alkyl, alkylene(hetero)cyclyl, (substituted) alkylenearyl, alkyleneheteroaryl; R3 = H, F, Cl, Br, OH, OR5, OCOR5, OCONHR5, etc.; A = alkylene, alkenediyl, alkyndiyl, etc.; B = COO2H, CO2R6, CONH2, CONHNH2, etc; Y = O, NH, NR5, NCOR5, NSO2R5, etc.; R5 = CF3, C2F5, (interrupted) (substituted) alkyl, alkenyl, alkynyl, etc.; R6 = (interrupted) alkyl, alkenyl, alkynyl, etc.], were prepd. for treatment of microglia-activation assocd. diseases such as inflammatory, allergic, infectious or autoimmune diseases. Thus, 500 mg Me 6-([2-benzylmercapto-1-(4-methylphenyl)-1H-benimidazol-6yl]oxy)hexanoate (prepn. given) in CH2Cl2 was stirred with m-ClPhCO(OOH) for 2 h at 20.degree. to give 232 mg 6-([1-(4-methylphenyl)-2-(phenylmethylsulfonyl)-1H-benimidazol-6-yl]oxy)hexanoic acid. The latter inhibited the microglia-activation with IC50 = 0.46 .mu.M. THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 18 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file req COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 3.25 168.71 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -0.65 -0.65

FILE 'REGISTRY' ENTERED AT 13:56:23 ON 11 MAR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7 DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

E11

1

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> e Pentanoic acid, 5-(4-(methylthio)phenoxy)-/cn PENTANOIC ACID, 1 5-(4-(IMINO(((PHENYLMETHOXY)CARBONYL)AMINO)M ETHYL) PHENOXY) -/CN 1 PENTANOIC ACID, 5-(4-(IMINO(((PHENYLMETHOXY)CARBONYL)AMINO)M . ETHYL) PHENOXY) -, ETHYL ESTER/CN E3 1 --> PENTANOIC ACID, 5-(4-(METHYLTHIO) PHENOXY)-/CN F.4 1 PENTANOIC ACID, 5-(4-ACETYL-2-ETHYL-5-HYDROXYPHENOXY)-2,2-DI METHYL-/CN E5 PENTANOIC ACID, 5-(4-ACETYL-2-METHOXYPHENOXY)-, METHYL ESTER /CN E6 PENTANOIC ACID, 5-(4-ACETYL-3-HYDROXY-2-PROPYLPHENOXY)-/CN . 1 PENTANOIC ACID, 5-(4-ACETYL-3-HYDROXY-2-PROPYLPHENOXY)-, E7 1 ETH YL ESTER/CN E8 PENTANOIC ACID, 5-(4-ACETYL-3-HYDROXY-2-PROPYLPHENOXY)-, 1 MET HYL ESTER/CN E9 PENTANOIC ACID, 5-(4-ACETYL-5-HYDROXY-2-(2-PROPENYL) PHENOXY) -/CN E10 PENTANOIC ACID, 5-(4-ACETYL-5-HYDROXY-2-PROPYLPHENOXY)-/CN 1

PENTANOIC ACID, 5-(4-ACETYLPHENOXY)-/CN

E12 1 PENTANOIC ACID, 5-(4-ACETYLPHENOXY)-, METHYL ESTER/CN

=> e3

L8 1 "PENTANOIC ACID, 5-(4-(METHYLTHIO)PHENOXY)-"/CN

=> d 18

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 485795-28-6 REGISTRY

CN Pentanoic acid, 5-[4-(methylthio)phenoxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H16 O3 S

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY 6.30 175.01 FULL ESTIMATED COST TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY SESSION 0.00 -0.65CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 13:57:02 ON 11 MAR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11 FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 18

L9 1 L8

=> d 19 ti fbib abs

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

TI Polyhydroxyalkanoate with (methylsulfanyl) phenoxy structure in side chain

AN 2003:40201 CAPLUS

DN 138:105715

TI Polyhydroxyalkanoate with (methylsulfanyl) phenoxy structure in side chain

IN Kenmoku, Takashi; Sugawa, Etsuko; Yano, Tetsuya; Imamura, Takeshi

PA Canon Kabushiki Kaisha, Japan

SO Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

GΙ

Ι

AB A polyhydroxyalkanoate that comprises a unit represented by the chem. formula (I): wherein n is an integer of 1-8 being the same or different in the polyhydroxyalkanoate. The microbial prodn. process is also disclosed.

=>

=>

Uploading 10025947 rce first action 2nd.str

=> file reg

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
5.75
180.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

-0.65
-1.30

FILE 'REGISTRY' ENTERED AT 14:01:36 ON 11 MAR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7 DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

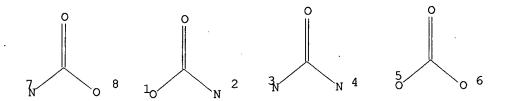
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10025947 rce first action 2nd.str

L10 STRUCTURE UPLOADED

=> d 110 L10 HAS NO ANSWERS L10 STF



G1 CH2, O,S, N, [@1-@2], [@3-@4], [@5-@6], [@7-@8] G2 O,S

Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

=> search 110 sss sam SAMPLE SEARCH INITIATED 14:02:26 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

> BATCH **INCOMPLETE**

EXCEEDS 1000000 PROJECTED ITERATIONS: PROJECTED ANSWERS: EXCEEDS 0

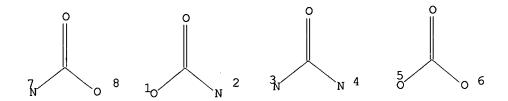
L11 0 SEA SSS SAM L10

=> Uploading 10025947 rce first action 2nd.str

STRUCTURE UPLOADED L12

=> d 112L12 HAS NO ANSWERS L12 STR

=>



G1 CH2,O,S,N,[@1-@2],[@3-@4],[@5-@6],[@7-@8] G2 O,S

Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

8 ANSWERS

=> search 112 sss sam
SAMPLE SEARCH INITIATED 14:04:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L13 0 SEA SSS SAM L12

=> search 112 sss full FULL SEARCH INITIATED 14:05:44 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 5.3% PROCESSED 400000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.22</pre>

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

L14

8 SEA SSS FUL L12

=> d scan

L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Carbamic acid, (4-phenylbutyl)-, phenylmethyl ester (9CI) IN

C18 H21 N O2 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

8 ANSWERS REGISTRY COPYRIGHT 2003 ACS D-Glucose, polymer with 5-phenoxypentanoic acid (9CI) IN

(C11 H14 O3 . C6 H12 O6)xMF

CI

CM 1

 $HO_2C-(CH_2)_4-OPh$

CM 2

Absolute stereochemistry.

8 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Cholest-5-en-3-ol (3.beta.)-, (4-phenylbutyl)carbamate (9CI) IN

C38 H59 N O2

Absolute stereochemistry.

L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Carbamic acid, (4-phenylbutyl)-, decyl ester (9CI)
MF C21 H35 N O2

$$O \\ || \\ Me - (CH2)9 - O - C - NH - (CH2)4 - Ph$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Adenosine, 2-chloro-2'-deoxy-, 5'-benzenehexanoate (9CI)
MF C22 H26 Cl N5 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Carbamic acid, (4-phenylbutyl)-, 1-phenylethyl ester (9CI)

MF C19 H23 N O2

$$\begin{array}{c|c} & \text{O} & \text{Ph} \\ & || & | \\ \text{Ph- (CH}_2)_4 - \text{NH- C- O- CH- Me} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN D-Glucose, polymer with 7-phenoxyheptanoic acid (9CI)

MF (C13 H18 O3 . C6 H12 O6)x

CI PMS

CM 1

$$HO_2C-(CH_2)_6-OPh$$

CM 2

Absolute stereochemistry.

L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Adenosine, 2'-deoxy-, 5'-benzenehexanoate (9CI)

MF C22 H27 N5 O4

Absolute stereochemistry.

ALL ANSWERS HAVE BEEN SCANNED

=> d cost		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
CONNECT CHARGES	3.06	16.81
NETWORK CHARGES	0.54	3.00
SEARCH CHARGES	147.75	303.94
DISPLAY CHARGES	0.00	7.96
	151.35	331.71
CAPLUS FEE (5%)	0.00	0.40
·		
FULL ESTIMATED COST	151.35	332.11
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

IN FILE 'REGISTRY' AT 14:06:52 ON 11 MAR 2003

=>

Uploading 10025947 rce first action 2nd.str

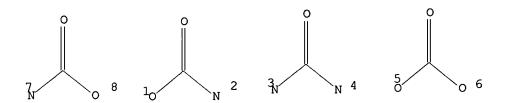
L15 STRUCTURE UPLOADED

STR

=> d 115

L15 HAS NO ANSWERS

L15



G1 CH2, O, S, N, [@1-@2], [@3-@4], [@5-@6], [@7-@8]

G2 0, S

G3 OH,SH

Structure attributes must be viewed using STN Express query preparation.

=> search 115 sss sam
SAMPLE SEARCH INITIATED 14:10:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

EXCEEDS 1000000

PROJECTED ANSWERS:

EXCEEDS

L16

0 SEA SSS SAM L15

=> logoff hold

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
153.75
334.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE SESSION 0.00 -1.30

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 14:10:50 ON 11 MAR 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1623paz

PASSWORD:

* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 14:14:18 ON 11 MAR 2003 FILE 'REGISTRY' ENTERED AT 14:14:18 ON 11 MAR 2003 COPYRIGHT (C) 2003 American Chemical Society (ACS)

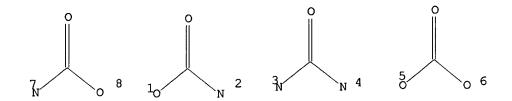
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
`	ENTRY	SESSION
FULL ESTIMATED COST	153.75	334.51
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

=>

Uploading 10025947 rce first action 2nd2.str

L17 STRUCTURE UPLOADED

=> d 117 , L17 HAS NO ANSWERS L17 STI



G1 CH2, O, S, N, [@1-@2], [@3-@4], [@5-@6], [@7-@8]

G2 0, S

G3 OH,SH

Structure attributes must be viewed using STN Express query preparation.

=> search 117 sss sam
SAMPLE SEARCH INITIATED 14:14:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 36404 TO ITERATE

2.7% PROCESSED 1000 ITERATIONS

0 ANSWERS

5 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 716721 TO 739439

PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> search 117 sss full FULL SEARCH INITIATED 14:15:10 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 722344 TO ITERATE

55.4% PROCESSED 400000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.07

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: PROJECTED ANSWERS:

722344 TO 722344 5 TO 18

L19

5 SEA SSS FUL L17

=> d scan

L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1-Hexadecanaminium, N,N,N-trimethyl-, salt with 11-phenoxyundecanoic acid (1:1) (9CI)

MF C19 H42 N . C17 H25 O3

CM 1

 $^{-02}C^{-}(CH_2)_{10}^{-}OPh$

CM 2

 $Me_3+N-(CH_2)_{15}-Me$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN D-Glucose, polymer with 7-phenoxyheptanoic acid (9CI)

MF (C13 H18 O3 . C6 H12 O6)x

CI PMS

CM 1

 $HO_2C-(CH_2)_6-OPh$

CM 2

Absolute stereochemistry.

L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Undecanoic acid, 11-phenoxy-, ion(1-) (9CI) IN

C17 H25 O3 MF

CI COM

 $-o_2C-(CH_2)_{10}-OPh$

L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS

D-Glucose, polymer with 5-phenoxypentanoic acid (9CI)

(C11 H14 O3 . C6 H12 O6)x MF

CI PMS

> CM 1

 HO_2C^- (CH₂)₄-OPh

2 CM

Absolute stereochemistry.

L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Dodecanoic acid, 12-phenoxy- (9CI)

MF C18 H28 O3

 $HO_2C-(CH_2)_{11}-OPh$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION

304.30 485.06 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

0.00 -1.30 CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 14:18:42 ON 11 MAR 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1623paz

PASSWORD:

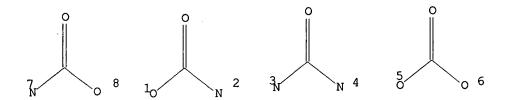
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 14:21:38 ON 11 MAR 2003 FILE 'REGISTRY' ENTERED AT 14:21:38 ON 11 MAR 2003 COPYRIGHT (C) 2003 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	304.30	485.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY 0.00	SESSION -1.30

Uploading 10025947 rce first action 2nd2.str

L20 STRUCTURE UPLOADED

=> d 120L20 HAS NO ANSWERS L20 STR



G1 CH2,O,S,N,[@1-@2],[@3-@4],[@5-@6],[@7-@8]

G2 0, S

G3 OH, SH

Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

=> search 120 sss sam
SAMPLE SEARCH INITIATED 14:22:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L21 0 SEA SSS SAM L20

=>

=>

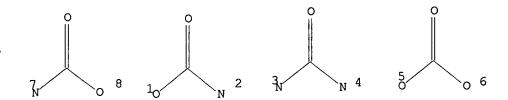
Uploading 10025947 rce first action 2nd2.str

L22 STRUCTURE UPLOADED

=> d 122

L22 HAS NO ANSWERS

L22 STR



G1 CH2,O,S,N,[@1-@2],[@3-@4],[@5-@6],[@7-@8]

G2 O, S

G3 OH, SH

Structure attributes must be viewed using STN Express query preparation.

2 ANSWERS

=> search 122 sss sam
SAMPLE SEARCH INITIATED 14:24:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 36403 TO ITERATE

2.7% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 716701 TO 739419

PROJECTED ANSWERS: 945 TO 1967

L23 2 SEA SSS SAM L22

=> d scan

L23 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Zincate(12-), (methyl
L-phenylalaninate-.kappa.N)[[4,4',4'',4'''-(21H,23H-

12 K⁺

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid, 5-[3-(1,1-dimethylethyl)-5-formyl-4-(2-propenyloxy)phenoxy]- (9CI)
MF C19 H26 O5

$$HO_2C-(CH_2)_4-O$$
 $Bu-t$
 $O-CH_2-CH=CH_2$
 CHO

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search 122 sss full FULL SEARCH INITIATED 14:24:48 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 722338 TO ITERATE

55.4% PROCESSED 400000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.12

1188 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

PROJECTED ITERATIONS: 722338 TO 722338

PROJECTED ANSWERS: 2007 TO 2283

L24 1188 SEA SSS FUL L22

=> d scan

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid,
5-[2-(1,1-dimethylethyl)-4-[[3-ethoxy-5,7-dihydro-7-imino2-[(methylamino)carbonyl]-6H-pyrrolo[3,4-b]pyridin-6-yl]acetyl]-6-[(2methoxyethyl)methylamino]phenoxy]-, monohydrobromide (9CI)
MF C32 H45 N5 O7 . Br H

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

HBr

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

REGISTRY COPYRIGHT 2003 ACS 1188 ANSWERS L24

Pentanoic acid, 5-[2-(dimethylamino)-6-(1,1-dimethylethyl)-4-[[5-ethoxy-IN 1,3-dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2yl]acetyl]phenoxy]-, monohydrobromide (9CI)

MF C31 H42 N4 O6 . Br H

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

● HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Octanoic acid, 8-[4-[[(1,2-dihydro-4-hydroxy-6-iodo-2-oxo-3-IN quinolinyl)carbonyl]amino]phenoxy]- (9CI)

C24 H25 I N2 O6 MF

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid, 5-(4-chloro-2-cyanophenoxy)- (9CI)
MF C12 H12 Cl N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6-[4-[(1E)-(4-hexylphenyl)azo]phenoxy]- (9CI)
MF C24 H32 N2 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS



IN Octanoic acid, 8-[2-[(methylamino)carbonyl]phenoxy]- (9CI)
MF C16 H23 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN L-Alanine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-, [4-(4-carboxybutoxy)phenyl](4-methylphenyl)methyl ester (9CI)
MF C37 H37 N O7

Absolute stereochemistry.

$$Me$$
 CC
 $CH_2)_4$
 Me
 Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Heptanoic acid, 7-[[5'-[[(8-phenyloctyl)amino]carbonyl]-3,3''-bis(trifluoromethyl)[1,1':3',1''-terphenyl]-2'-yl]oxy]- (9CI)
MF C42 H45 F6 N O4



L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Octanoic acid, 8-[2-(aminooxoacetyl)-5-phenoxyphenoxy]- (9CI)
MF C22 H25 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT



L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Hexanoic acid, 6-[2-[[4-[[(4'-amino[1,1'-biphenyl]-2-

yl)carbonyl]amino]benzoyl]methylamino]-5-methylphenoxy]- (9CI)

MF C34 H35 N3 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Undecanoic acid, 11,11'-[carbonylbis[(2-iodo-4,1-phenylene)oxy]]bis(9CI)
MF C35 H48 I2 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Octanoic acid,

MF C23 H28 N2 O5

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid, 5-[3-(1,1-dimethylethyl)-4-hydroxy-5-[[[(1S,2S)-2-[[(4-methylphenyl)sulfonyl]amino]cyclohexyl]imino]methyl]phenoxy]- (9CI)
MF C29 H40 N2 O6 S

Absolute stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid,

5-[2-(2-cyanoethyl)-6-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-

dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]phenoxy], monohydrobromide (9CI)

MF C32 H40 N4 O6 . Br H

$$\begin{array}{c|c} & \text{NC-CH}_2\text{-CH}_2 \\ & \text{O} & \text{O-(CH}_2)_4\text{-CO}_2\text{H} \\ & \text{D} & \text{O} \\ & \text{O} & \text{O} \end{array}$$

HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid,

5-[2-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]-6-(1-pyrrolidinyl)phenoxy]- (9CI)

MF C33 H44 N4 O6

CI COM

$$\begin{array}{c|c}
 & \text{T-Bu} \\
 & \text{O} \\
 & \text{NH} \\
 & \text{O} \\
 & \text{CH}_2 - \text{C}
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6,6'-[2,3-naphthalenediylbis(oxy)]bis- (9CI)
MF C22 H28 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6,6'-[1,2-phenylenebis(oxy)]bis- (9CI)
MF C18 H26 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid,
6-[2-[[[(4-chlorophenyl)sulfonyl]hydrazono]methyl]phenoxy](9CI)
MF C19 H21 C1 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24

1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
Zincate(12-), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24) tetrakis[3,5-bis(4-1.14)] IN carboxybutoxy)benzoato]](14-)](3-pyridinecarboxamide-.kappa.N1)-, dodecapotassium, (SP-5-21) - (9CI)

C94 H86 N6 O33 Zn . 12 K MF

CCS CI

PAGE 1-A

$$CO_2^ CO_2^ CO_2^-$$

●12 K⁺

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Heptanoic acid, 7-[(5,9,10,14-tetraethyl-21-methoxy-4,15-dimethyl-8,11-imino-3,6:16,13-dinitrilo-1,18-benzodiazacycloeicosin-20-yl)oxy]- (9CI)
MF C40 H49 N5 O4

$$Me$$
 Et
 $HO_2C-(CH_2)_6-O$
 N
 HN
 HN
 Et
 Me
 Et

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Hexanoic acid, 6-[2-[[4-[(2-aminobenzoyl)amino]benzoyl]methylamino]-5-methylphenoxy]- (9CI)

MF C28 H31 N3 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

Absolute stereochemistry.

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS IN Dodecanoic acid, 12-(4-fluorophenoxy)- (9CI) MF C18 H27 F O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6-[4-(methylthio)phenoxy]- (9CI)
MF C13 H18 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid, 5-[2-(1-cyano-1-methylethyl)-4-[[3-ethoxy-5,7-dihydro-7imino-2-[(methylamino)carbonyl]-6H-pyrrolo[3,4-b]pyridin-6yl]acetyl]phenoxy]-, monohydrobromide (9CI)

MF C28 H33 N5 O6 . Br H

MeNH-C NH O (CH₂)
$$_4$$
 - CO₂H EtO

HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid,

5-[2-(diethylamino)-6-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-dihydro-1-imino-5,6-dimethoxy-2H-isoindol-2-yl)acetyl]phenoxy]-,
monohydrobromide (9CI)

MF C31 H42 F N3 O6 Br H

MeO
$$\begin{array}{c} \text{NEt2} \\ \text{O- (CH2)}_4 - \text{CO}_2\text{H} \\ \text{Bu-t} \end{array}$$

HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Octanoic acid, 8-[4-[[(2,5-dihydro-4-hydroxy-5-methyl-2-oxo-1-phenyl-1H-pyrrol-3-yl)carbonyl]amino]phenoxy]- (9CI)
MF C26 H30 N2 O6

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .alpha.-D-Glucopyranoside, methyl 2-[[[2-[(5-carboxypentyl)oxy]-4,6-dimethoxyphenyl]methyl]amino]-2-deoxy-3,6-bis-O-(phenylmethyl)- (9CI)
MF C36 H47 N O10

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Octanoic acid, 8-[2-[(2-hydroxybenzoyl)amino]phenoxy]- (9CI)
MF C21 H25 N O5

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6-[(2,2',4',5'-tetrachloro[1,1'-biphenyl]-4-yl)oxy]- (9CI)
MF C18 H16 C14 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Absolute stereochemistry.

Me
$$CC$$
 $CCH_2)$ 7
 $CCH_2)$ 7
 $CCH_2)$ 8
 $CCH_2)$ 8
 $CCH_2)$ 8
 $CCH_2)$ 9
 $CCH_2)$ 7
 $CCH_2)$ 9
 $CCH_2)$ 7
 $CCH_2)$ 7
 $CCH_2)$ 9
 $CCH_2)$ 7
 $CCH_2)$ 9
 C

PAGE 1-A

CHMe2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Undecanoic acid, 11-(3,4-dimethoxyphenoxy)- (9CI)
MF C19 H30 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid, 5-(4-formyl-3-hydroxyphenoxy)- (9CI)
MF C12 H14 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid, 5-[4-[[4-(dodecyloxy)phenyl]azo]phenoxy]- (9CI)
MF C29 H42 N2 O4

$$N = N$$

$$O = (CH2)11 - Me$$

$$N = N$$
 $O - (CH2)4 - O$
 $O - (CH2)11 - Me$

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1-Hexadecanaminium, N,N,N-trimethyl-, salt with 11,11'-[1,3phenylenebis(oxy)]bis[undecanoic acid] (2:1) (9CI)

MF C28 H44 O6 . 2 C19 H42 N

CM 1

CM 2

 $Me_3+N-(CH_2)_{15}-Me$

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6-[4-[2-[4-(decylsulfonyl)phenyl]ethenyl]phenoxy]- (9CI)
MF C30 H42 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Dodecanoic acid, 12-[2-[(3-carboxypropyl)thio]phenoxy]- (9CI)
MF C22 H34 O5 S

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Pentanoic acid, 5-[2-[3-(cyanomethyl)-1-pyrrolidinyl]-4-[(2-cyclopropyl-5,7-dihydro-7-imino-6H-pyrrolo[3,4-b]pyridin-6-yl)acetyl]-6-(1,1-dimethylethyl)phenoxy]-, monohydrobromide (9CI)

MF C33 H41 N5 O4 . Br H

NH NH
$$CH_2$$
 C CH_2 CH_2 CH_2 CH_2 CH_2 CH_2

• HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid,
5-[2-(1,1-dimethylethyl)-4-[[2-(fluoromethyl)-5,7-dihydro-

7-imino-6H-pyrrolo[3,4-b]pyridin-6-yl]acetyl]-6-(1-pyrrolidinyl)phenoxy]-, monohydrobromide (9CI)
MF C29 H37 F N4 O4 . Br H

• HBr

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Undecanoic acid, 11-[4-[(4-butylphenyl)azo]phenoxy]- (9CI)

MF C27 H38 N2 O3

CI COM

$$N = N$$
 $Bu-n$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Absolute stereochemistry.

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS IN Octanoic acid, 8-(2-methoxyphenoxy)- (9CI) MF C15 H22 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PAGE 1-A

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 3-Pyridinecarboxylic acid,
6-[[3-[(7-carboxyheptyl)oxy]-5,6,7,8-tetrahydro5,5,8,8-tetramethyl-2-naphthalenyl]seleno]- (9CI)
MF C28 H37 N O5 Se

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid,
5-[2-(aminooxoacetyl)-5-([1,1'-biphenyl]-3-yloxy)phenoxy](9CI)
MF C25 H23 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid, 5-[5-[(3-amino-2-pyridinyl)amino]-2-[[(4-chlorophenyl)sulfonyl]amino]phenoxy]- (9CI)
MF C22 H23 Cl N4 O5 S

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp 124 histcmpds2a/ HISTCMPDS2A/ IS NOT A VALID SAVED NAME Enter the name you wish to use for the saved query, answer set, or L-number list. The name must:

- 1. Begin with a letter,
- 2. Have 1-12 characters,
- 3. Contain only letters (A-Z) and numbers (0-9),
- 4. End with /Q for a query (search profile, structure, or screen set), /A for an answer set, or /L for an L-number list.
- 5. Not already be in use as a saved name,

```
6. Not be END, SAV, SAVE, SAVED
  7. Not have the form of an L-number (Lnnn).
ENTER NAME OR (END):histcmpds2/a
ANSWER SET L24 HAS BEEN SAVED AS 'HISTCMPDS2/A'
=> e Hexanoic acid, 6,6'-(1,2-phenylenebis(oxy))bis-/cn
MISMATCHED QUOTE IN EXPAND TERM
Quotation marks (or apostrophes) must be used in pairs,
one before and one after the expression you are setting
off or masking.
=> e Undecanoic acid, 11-(3,4-dimethoxyphenoxy)-/cn
                  UNDECANOIC ACID, 11-(2-THIAZOLIN-2-YLAMINO)-, PICRATE/CN
             1
                   UNDECANOIC ACID, 11-(3,4-DIHYDROXYPHENYL)-, METHYL ESTER/CN
E2
             1 --> UNDECANOIC ACID, 11-(3,4-DIMETHOXYPHENOXY)-/CN
E3
                   UNDECANOIC ACID, 11-(3,4-XYLYL)-, METHYL ESTER/CN
E4
             1
             1
                   UNDECANOIC ACID,
E.5
11-(3-((((2,2-DIMETHYL-1,3-DIOXOLAN-4-YL)ME
                   THOXY) HYDROXYPHOSPHINYL) OXY) -2-METHOXYPROPOXY) -,
(S-(R^*,S^*))
                    -/CN
             1
                    UNDECANOIC ACID,
11-(3-((HYDROXY(2-(4-NITROPHENYL)ETHOXY)PHO
                    SPHINYL)OXY)-2-METHOXYPROPOXY)-, (R)-/CN
                   UNDECANOIC ACID, 11-(3-(1-ADAMANTYL)UREIDO)-/CN UNDECANOIC ACID, 11-(3-(1-ADAMANTYL)UREIDO)-,
             1
E8
3-(DIMETHYLAMI
                   NO) PROPYL ESTER/CN
                   UNDECANOIC ACID, 11-(3-(1-ADAMANTYL)UREIDO)-, ETHYL
F.9
             1
ESTER/CN
             1
                   UNDECANOIC ACID,
E10
11-(3-(10,15,20-TRIS(4-METHYLPHENYL)-21H,23
                   H-PORPHIN-5-YL) PHENOXY) -/CN
             1
                   UNDECANOIC ACID,
11-(3-(10,15,20-TRIS(4-METHYLPHENYL)-21H,23
                    H-PORPHIN-5-YL) PHENOXY) -, METHYL ESTER/CN
                    UNDECANOIC ACID,
11-(3-(2-(3-(HYDROXYMETHYL)-4-OXO-2-OXETANY
                    L) ETHYL) PHENOXY) -, METHYL ESTER, TRANS-/CN
=> e3
L25
             1 "UNDECANOIC ACID, 11-(3,4-DIMETHOXYPHENOXY)-"/CN
=> d 125
L25 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
     227291-94-3 REGISTRY
RN
     Undecanoic acid, 11-(3,4-dimethoxyphenoxy)- (9CI) (CA INDEX
CN
     NAME)
FS
     3D CONCORD
MF
     C19 H30 O5
SR
     CA
```

STN Files: CA, CAPLUS

LC

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file ca[lus
'CAOLUS' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'REGISTRY'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available. If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue

accessing the remaining file names entered.

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 643.91 FULL ESTIMATED COST 463.15 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION 0.00 -1.30CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11 FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 125 L26

1 L25

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
     Preparation of arylalkanoic acids and analogs as fibroblast growth factor
     receptor antagonists
     1999:388146 CAPLUS
AN
     131:44430
DN
     Preparation of arylalkanoic acids and analogs as fibroblast growth factor
ΤI
     receptor antagonists
     Chan, Ming Fai; Balaji, Vitukudi Narayanaiyengar; Ramnarayan,
IN
     Kalyanaraman; Schove, Laura; Castillo, Rosario Silvestre; Kois, Adam
PA
     Eisai Co., Ltd., Japan
     PCT Int. Appl., 155 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                       KIND DATE
                                             APPLICATION NO. DATE
                       ____
                       A2
                              19990617
                                              WO 1998-US25789 19981204
PΙ
     WO 9929640
                       A3
                              20000113
     WO 2000029640
             AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
              DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE,
              KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW,
             MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
MT
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
              CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                              US 1997-986248
                                                                 19971205
                                              US 1998-79343
                                                                 19980515
     AU 9919037
                        A1
                              19990628
                                              AU 1999-19037
                                                                 19981204
                                              US 1997-986248
                                                                 19971205
                                              US 1998-79343
                                                                 19980515
                                              WO 1998-US25789
                                                                19981204
     MARPAT 131:44430
OS
     RZZ1R1 [I; R = (un)substituted (hetero)aryl; R1 = CO2H, B(OH)2, SO3H,
AB
     P(O)(OH)2; Z = bond, O, NH, CO, alkenylene, etc.; Z1 = alkylene, arylene,
     O, NH, etc.] were prepd. Thus, 4-IC6H4OCH2CO2H was condensed with
     PhC.tplbond.CH to give 4-(PhC.tplbond.C)C6H4OCH2CO2H. Data for biol.
     activity of I were given.
=> fil;e reg
                                                     SINCE FILE
COST IN U.S. DOLLARS
                                                                      TOTAL
                                                          ENTRY
                                                                    SESSION
                                                            4.08
                                                                      647.99
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                     SINCE FILE
                                                                      TOTAL
                                                          ENTRY
                                                                    SESSION
```

-0.65

-1.95

FILE 'HOME' ENTERED AT 14:32:16 ON 11 MAR 2003

CA SUBSCRIBER PRICE

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

The EXPAND command is used to look at the index in a file which has an index. This file does not have an index.

=> file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 0.21 648.20 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION 0.00 -1.95CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7 DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

```
=> e Octanoic acid, 8-(2-methoxyphenoxy)-/cn
                   OCTANOIC ACID, 8-(2-ISOINDOLINYL)-/CN
             1
                   OCTANOIC ACID, 8-(2-METHOXYETHOXY)-/CN
E2
             1 --> OCTANOIC ACID, 8-(2-METHOXYPHENOXY)-/CN
E3
E4
             1
                   OCTANOIC ACID, 8-(2-METHYLPHENOXY)-/CN
                   OCTANOIC ACID, 8-(2-NAPHTHALENYLAMINO)-8-OXO-, METHYL
E5
ESTER/
                   OCTANOIC ACID, 8-(2-NAPHTHALENYLOXY)-, ETHYL ESTER/CN
F.6
                   OCTANOIC ACID, 8-(2-NAPHTHALENYLTHIO)-2-OXO-, METHYL
E7
ESTER/C
                   OCTANOIC ACID, 8-(2-NAPHTHOYL)-/CN
E8
             1
                   OCTANOIC ACID, 8-(2-NITROPHENOXY)-/CN
F.9
             1
                   OCTANOIC ACID, 8-(2-OXOCYCLOPENTYLIDENE)-/CN
E10
            1
                   OCTANOIC ACID, 8-(2-OXOCYCLOPENTYLIDENE)-, METHYL ESTER/CN
E11
            1
                   OCTANOIC ACID, 8-(2-PROPENYLOXY)-/CN
E12
            1
=> e3
             1 "OCTANOIC ACID, 8-(2-METHOXYPHENOXY)-"/CN
L27
```

L27 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 338994-29-9 REGISTRY

CN Octanoic acid, 8-(2-methoxyphenoxy)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H22 O4

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION 654.50 FULL ESTIMATED COST 6.30 TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY SESSION 0.00 -1.95CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11 FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 127

L28 1 L27

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
     Preparation of phenoxyalkanoic acids as drug delivery agents
ΤI
     2001:338472 CAPLUS
AN
DN
     134:353172
     Preparation of phenoxyalkanoic acids as drug delivery agents
ΤI
     Leone-Bay, Andrea; Kraft, Kelly; Moye-Sherman, Destardi; Gschneidner,
IN
     David; Boyd, Maria A. P.; Liu, Puchun; Tang, Pinwah; Liao, Jun; Smarth,
     John E.; Freeman, John J., Jr.
     Emisphere Technologies, Inc., USA
PA
     PCT Int. Appl., 107 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LА
FAN.CNT 2
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
                           -----
                                           _____
                                                            _____
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PΙ
     WO 2001032596
                      A1
                            20010510
                                           WO 2000-US30662 20001106
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                                           US 2000-237233PP 20001002
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PATENT FAMILY INFORMATION:
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                           DATE
                                           APPLICATION NO. DATE
     WO 2001032130
                      A2
                            20010510
                                           WO 2000-US41960 20001106
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             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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US 1999-163806PP 19991105 US 2000-231836PP 20000906 US 2000-237233PP 20001002 Α5 20010514 AU 2001-26223 20001106 AU 2001026223 US 1999-163806PP 19991105 US 2000-231836PP 20000906 US 2000-237233PP 20001002 WO 2000-US41960W 20001106 EP 1226109 A2 20020731 EP 2000-989761 20001106 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR US 1999-163806PP 19991105 US 2000-231836PP 20000906 US 2000-237233PP 20001002 WO 2000-US41960W 20001106 MARPAT 134:353172

AΒ R10Z1Z2CO2H [I; R1 = (un) substituted Ph; Z1 = (heteroatom-interrupted) alk(en)ylene or (hetero)arylene; Z2 = bond, (hydroxy)arylene, haloarylene]

were prepd. Thus, 2-(HO)C6H4OCH2Ph was etherified by Br(CH2)6CO2Et and the product deprotected to give 2-(HO)C6H4O(CH2)6CO2H. Data for drug delivery activity of I were given.

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 11 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold TOTAL COST IN U.S. DOLLARS SINCE FILE ENTRY SESSION FULL ESTIMATED COST 10.12 664.62 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -0.65 -2.60CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 14:35:14 ON 11 MAR 2003

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NEWS Apr 09 ZDB will be removed from STN 4

NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and **IFIUDB**

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NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and
ZCAPLUS
NEWS 7
                 BIOSIS Gene Names now available in TOXCENTER
         Apr 22
NEWS 8
         Apr 22
                 Federal Research in Progress (FEDRIP) now available
NEWS 9
         Jun 03
                 New e-mail delivery for search results now available
NEWS 10
         Jun 10
                 MEDLINE Reload
NEWS 11
         Jun 10
                 PCTFULL has been reloaded
         Jul 02
                 FOREGE no longer contains STANDARDS file segment
NEWS 12
NEWS 13
         Jul 22 USAN to be reloaded July 28, 2002;
                 saved answer sets no longer valid
         Jul 29
NEWS 14
                 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08
                 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
                 now available on STN
                 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 20 Aug 19
NEWS 21 Aug 19
                 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26
                 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03
                 JAPIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
         Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 25
NEWS 26 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27
         Oct 21 EVENTLINE has been reloaded
NEWS 28 Oct 24 BEILSTEIN adds new search fields
NEWS 29
        Oct 24 Nutraceuticals International (NUTRACEUT) now available on
STN
NEWS 30 Oct 25 MEDLINE SDI run of October 8, 2002
NEWS 31 Nov 18 DKILIT has been renamed APOLLIT
NEWS 32 Nov 25
                 More calculated properties added to REGISTRY
NEWS 33 Dec 02 TIBKAT will be removed from STN
NEWS 34 Dec 04 CSA files on STN
NEWS 35 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36 Dec 17 TOXCENTER enhanced with additional content
NEWS 37 Dec 17 Adis Clinical Trials Insight now available on STN
NEWS 38 Dec 30 ISMEC no longer available
NEWS 39 Jan 13 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40 Jan 21 NUTRACEUT offering one free connect hour in February 2003
NEWS 41 Jan 21
                PHARMAML offering one free connect hour in February 2003
NEWS 42 Jan 29 Simultaneous left and right truncation added to COMPENDEX,
                 ENERGY, INSPEC
NEWS 43 Feb 13 CANCERLIT is no longer being updated
NEWS 44 Feb 24 METADEX enhancements
NEWS 45 Feb 24 PCTGEN now available on STN
NEWS 46 Feb 24 TEMA now available on STN
NEWS 47 Feb 26 NTIS now allows simultaneous left and right truncation
NEWS 48 Feb 26 PCTFULL now contains images
NEWS 49 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results
              January 6 CURRENT WINDOWS VERSION IS V6.01a,
NEWS EXPRESS
              CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
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=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7 DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 10025947 rce first action 2nd3.str

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

50 ANSWERS

=> search 11 sss sam
SAMPLE SEARCH INITIATED 07:26:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 516 TO ITERATE

100.0% PROCESSED 516 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8958 TO 11682

PROJECTED ANSWERS: 931 TO 1949

L2 50 SEA SSS SAM L1

=> d scan

G1 O, S, N

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[3-[2-(1-methyl-1H-benzimidazol-2-

yl)ethenyl]phenyl]amino]-4-oxo-, monosodium salt (9CI)

MF C20 H17 N3 O3 . Na

Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 2,5-bis[[[4-[[4-[(3-carboxy-1-oxo-2-propenyl)amino]phenyl]sulfonyl]phenyl]amino]carbonyl]-, (Z,Z)- (9CI)

MF C41 H30 N4 O14 S2

Double bond geometry as shown.

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[4-(aminoiminomethyl)phenyl]amino]-4-oxo-, (E)- (9CI)

MF C11 H11 N3 O3

CI COM

Double bond geometry as shown.

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[(5-chloro-2-hydroxyphenyl)amino]-4-oxo- (9CI)

MF C10 H8 Cl N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[4-[[(4-methoxyphenyl)amino]sulfonyl]phenyl]amino]-4-

oxo- (9CI)

MF C17 H16 N2 O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS - REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[(2-chlorophenyl)amino]-4-oxo-, (E)- (9CI)

MF C10 H8 C1 N O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[3-[2-(4-ethyl-5-methyl-2-thiazolyl)ethenyl]phenyl]amino]-4-oxo-, monosodium salt, (E,Z)- (9CI) MF C18 H18 N2 O3 S . Na

Double bond geometry as shown.

Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4,4'-[1,4-phenylenebis[(dicyanoethenylidene)imino-4,1-phenyleneoxy-4,1-phenyleneimino]]bis[4-oxo-, (Z,Z)-, homopolymer (9CI)

MF (C46 H30 N8 O8)x

CI PMS

CM 1

Double bond geometry as shown.

PAGE 1-B

IN 2-Butenoic acid, 4-[[7-[[5-[[[[[3-[[[[6-[[8-[(3-carboxy-1-oxo-2-propenyl)amino]-1-hydroxy-3,5-disulfo-2-naphthalenyl]azo]-5-sulfo-1-naphthalenyl]methyl]amino]carbonyl]amino]methyl]-3,5,5-

REGISTRY COPYRIGHT 2003 ACS

naphthalenyl]methyl]amino]carbonyl]amino]methyl]-3,5,5trimethylcyclohexyl]amino]carbonyl]amino]methyl]-1-sulfo-2naphthalenyl]azo]-8-hydroxy-4,6-disulfo-1-naphthalenyl]amino]-4-oxo-,
[2Z(2Z)]- (9CI)

MF C62 H58 N10 O28 S6

50 ANSWERS

L2

Double bond geometry as described by E or Z.

PAGE 1-B

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[5-[4-[(3-carboxy-1-oxo-2-propenyl)amino]benzoyl]-2-methylphenyl]amino]-4-oxo- (9CI)

MF C22 H18 N2 O7

$$O HO_2C-CH = CH-C-NH$$
 $O HO_2C-CH = CH-C-NH$
 $O HO_2C-CH = CH-C-NH$
 $O HO_2C-CH = CH-C-NH$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[4-[3-(decylamino)-3-oxo-2-phenyl-1-propenyl]phenyl]amino]-4-oxo-, (Z,E)- (9CI)

MF C29 H36 N2 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS IN Maleanilic acid, 2'-hydroxy-, acetate (6CI) MF C12 H11 N O5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Butenoic acid, 4-oxo-4-[[4-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)oxy]phenyl]amino]-, (Z)- (9CI)
MF C18 H12 F13 N O4

Double bond geometry as shown.

$$F_3C$$
 (CF₂)₅ O CO₂H

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenedioic acid (2Z)-, mono[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl]
ester (9CI)

MF C35 H50 O5 S2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[(2-iodophenyl)amino]-4-oxo- (9CI)

MF C10 H8 I N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Butenoic acid, 4,4'-[(5-hydroxy-1,3-phenylene)diimino]bis[4-oxo-,(Z,Z)-

(9CI) MF C14 H12 N2 O7

Double bond geometry as shown.

$$Z$$
 CO_2H
 O
 CO_2H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[3-[2-(4-heptyl-2-thiazolyl)ethenyl]phenyl]amino]-4-oxo-, monosodium salt, (E,Z)- (9CI)

MF C22 H26 N2 O3 S . Na

Double bond geometry as shown.

Na

- L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
- IN Cobalt, diaqua[[4,4'-[methylenebis(4,1-phenyleneimino)]bis[4-oxo-2-butenoato]](2-)-O1,O4]- (9CI)
- MF C21 H20 Co N2 O8
- CI CCS

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, $4-\infty-4-[(4-\text{sulfophenyl})\text{amino}]-$, disodium salt, (2)-, polymer with

(Z,Z)-.alpha.-(4-amino-1,4-dioxo-2-butenyl)-.omega.-[(4-amino-1,4-dioxo-2-butenyl)oxy]poly[oxy(methyl-1,2-ethanediyl)], 2,5-furandione and .alpha.-2-propenyl-.omega.-hydroxypoly(oxy-1,2-ethanediyl) (9CI)

MF (C10 H9 N O6 S . C4 H2 O3 . (C3 H6 O) n C8 H8 N2 O5 . (C2 H4 O) n C3 H6 O . 2 Na) x

CI PMS, COM

CM 1

CM 2

Double bond geometry as shown.

●2 Na

CM 3

$$HO \longrightarrow CH_2 - CH_2 - O \longrightarrow CH_2 - CH \longrightarrow CH_2$$

CM 4

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[4-(difluoromethoxy)phenyl]amino]-4-oxo- (9CI)

MF C11 H9 F2 N O4

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{NH-C-CH} = \text{CH-CO}_2\text{H} \\ \\ \text{F}_2\text{CH-O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading 10025947 rce first action 2nd3.str

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

G1 O, S, N

G1 O, S, N

Structure attributes must be viewed using STN Express query preparation.

=> search 13 sss sam SAMPLE SEARCH INITIATED 07:29:09 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 516 TO ITERATE

100.0% PROCESSED 516 ITERATIONS SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 8958 TO 11682

PROJECTED ANSWERS:

1 TO

1 SEA SSS SAM L3 L4

=> d scan

1 ANSWERS REGISTRY COPYRIGHT 2003 ACS

2-Butenoic acid, 4-(4-chloro-2-methylphenoxy)-, ammonium salt (9CI)

MF C11 H11 C1 O3 . H3 N

€НИ ●

```
=> e 2-Butenoic acid, 4-(4-chloro-2-methylphenoxy)-, ammonium salt/cn
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-,
E1
2-ETHOXYETHY
                   L ESTER/CN
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, 2-PROPENYL
E2
Ε
                   STER/CN
             1 --> 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, AMMONIUM
E3
SAL
                   T/CN
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, BUTYL
E4
             1
ESTER/
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, COMPD.
E5
             1
WITH
                   N-METHYLMETHANAMINE (1:1)/CN
F.6
             1
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, ETHYL
ESTER/
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, METHYL
E7
             1
ESTER
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, PROPYL
E.8
             1
ESTER
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, SODIUM
E9
             1
SALT/
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-3-ETHOXY-,
E10
             1
ETH
                   YL ESTER, (E)-/CN
                   2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENYL)-4-OXO-,
E11
             1
(2E) - / C
                   2-BUTENOIC ACID,
E12
             1
4-(4-CHLORO-3-METHOXY-5-(METHYLAMINO) PHENYL
                   )-3-METHYL-, METHYL ESTER, (E)-/CN
=> e3
L5
             1 "2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, AMMONIUM
SALT"/
               CN
=> d 15
    ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
     68838-73-3 REGISTRY
RN
     2-Butenoic acid, 4-(4-chloro-2-methylphenoxy)-, ammonium salt
           (CA INDEX NAME)
     (9CI)
MF
    C11 H11 C1 O3 . H3 N
LC
     STN Files:
                 CA, CAPLUS
CRN (68838-71-1)
```

● инз .

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 9.90 10.11

FULL ESTIMATED COST

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FILE COVERS 1907 - 12 Mar 2003 VOL 138 ISS 11 FILE LAST UPDATED: 11 Mar 2003 (20030311/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 15

L6 1 L5

=> d 16 ti fbib abs

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

TI Phenoxycrotonate herbicidal compounds

AN 1979:34995 CAPLUS

DN 90:34995

TI Phenoxycrotonate herbicidal compounds

IN Sadohara, Hideo; Yamauchi, Sanji; Sugiyama, Hidetoshi; Takayama, Shuichi

PA Kumiai Chemical Industry Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	JP 53101527	A2	19780905	JP 1977-16837	19770217
				JP 1977-16837	19770217

GΙ

$$C1$$
 OCH₂CH= CHCO₂H

AB Phenoxycrotonates I (X = Cl or Me) or their alkyl esters, salts, or amides

are herbicides. Thus, 4-(2',4'-dichlorophenoxy)crotonic acid [17592-43-7] at 100 g/10 are completely killed Eleocharis acicularia, Cyperus serotinus, Sagittaria pygmaea, Scirpus juncoides, arrowhead, Echinochloa, Monochoria vaginalis, and Cyperus diformia infested in rice fields.

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	4.08	14.19
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.65	-0.65

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:34:46 ON 12 MAR 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1623paz

* * * * * *

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS Web Page URLs for STN Seminar Schedule - N. America NEWS BLAST(R) searching in REGISTRY available in STN on the Web Jan 25 NEWS Jan 25 Searching with the P indicator for Preparations NEWS 4 Jan 29 FSTA has been reloaded and moves to weekly updates DKILIT now produced by FIZ Karlsruhe and has a new update NEWS 5 Feb 01 frequency Access via Tymnet and SprintNet Eliminated Effective 3/31/02 Feb 19 NEWS - 6 Gene Names now available in BIOSIS Mar 08 NEWS 7 Mar 22 TOXLIT no longer available NEWS 8 TRCTHERMO no longer available NEWS 9 Mar 22 NEWS 10 Mar 28 US Provisional Priorities searched with P in CA/CAplus and USPATFULL NEWS 11 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY PAPERCHEM no longer available on STN. Use PAPERCHEM2 NEWS 12 Apr 02 instead. NEWS 13 Apr 08 "Ask CAS" for self-help around the clock

Welcome to STN International

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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^{*}LBEILSTEIN - BEILSTEIN Learning File

^{*} The files listed above are temporarily unavailable.

FILE 'HOME' ENTERED AT 13:17:15 ON 08 APR 2002

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 13:17:30 ON 08 APR 2002
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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5 DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

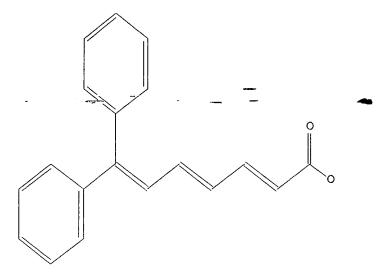
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Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

Uploading 10025947 elected specie.str

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 ssssam

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> search 11 sss sam
SAMPLE SEARCH INITIATED 13:18:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 0 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 4 TO 200

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search 11 sss full FULL SEARCH INITIATED 13:18:15 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 144 TO ITERATE

100.0% PROCESSED 144 ITERATIONS 2 ANSWERS SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> d scan

L3 2 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6-Heptatrienoic acid,
3-methyl-7-phenyl-7-(1,2,3,4-tetrahydro-1-methyl-6-quinolinyl)-, (2E,4E,6Z)- (9CI)
MF C24 H25 N O2

Double bond geometry as shown.

$$\begin{array}{c|c} & \text{Me} \\ & \\ \text{HO}_2\text{C} & \text{E} & \text{E} \\ & \\ & \text{Ph} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 2 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6-Heptatrienoic acid,
3-methyl-7-phenyl-7-(1,2,3,4-tetrahydro-1-methyl6-quinolinyl)-, (all-E)- (9CI)
MF C24 H25 N O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 141.04 141.25

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 13:19:29 ON 08 APR 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 8 Apr 2002 VOL 136 ISS 15 FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 13 L4

=> d l4 ti fbib abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

TI Preparation of heterocyclic compounds and mono- or polyenic carboxylic acid derivatives having potent binding activity to retinoid receptors

AN 1996:469506 CAPLUS

1 L3

DN 125:114703

TI Preparation of heterocyclic compounds and mono- or polyenic carboxylic acid derivatives having potent binding activity to retinoid receptors

IN Hibi, Shigeki; Kikuchi, Kouichi; Yoshimura, Hiroyuki; Nagai, Mitsuo; Tagami, Katsuya; Abe, Shinya; Hishinuma, Ieharu; Nagakawa, Junichi; Miyamoto, Norimasa; et al.

PA Eisai Co., Ltd., Japan

SO PCT Int. Appl., 203 pp. CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 3

RW: AU, CA, CN, FI, HU, KR, MX, NO, NZ, RU, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

JP 1994-267287 A 19941031

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JP 1995-166120 A 19950630
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                            DATE
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20001017
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FAN
    1996:601252
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                            DATE
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                      ____
                            _____
                                           ______
                                                            _____
ΡI
     JP 08188857
                       A2
                            19960723
                                           JP 1995-208140
                                                            19950815
                                           JP 1994-276287 A 19941110
OS
     MARPAT 125:114703
GI
     For diagram(s), see printed CA Issue.
     Novel retinoid-related compds. represented by the general formula
AΒ
     Z-(CR3:CR2)nCO2R1 [R1 = H, CO2H-protecting group; R2, R3 = H, halo,
linear
     or branched lower alkyl, linear or branched lower alkoxy, aryl; n = 1-3;
n
     no. of R2 or R3 are same or different; Z = heterocyclyl such as Q, Q1,
and
     Q2; A, B, D = CH, N, S, or S; E = CH, N; F, G = CH, N, S, O; wherein X1,
     X2, Y1, Y2 = H, NR4R5, CR6R7R8, OR9, S(O)mR10 (m = 0,1,2); wherein R6 -
     R12 = H, linear or branched alkyl; or X1 and Y2 or X2 and Y2 together
with
     the C atoms to which they are bonded form an (un)satd. and
(un) substituted
     ring optionally contg. O, S, or N; X3, Y3 = H, linear or branched alkyl
or
     alkoxy, cycloalkyl, aryl, heteroaryl, fluoroalkyl, halo; provided that Z
     .noteq. Ph, 2-naphthyl, etc.] and heterocyclic compds. [I; R1, R2 = H,
     lower alkyl, alkenylalkyl, alkynylalkyl, cycloalkyl, cycloalkylalkyl,
     lower alkoxyalkyl, aryl, heteroaryl, arylalkyl; or R1 and R2 together
form
     a cycloalkyl ring contg. S, O, SO, SO, NH, or alkylimino; ring A = Q3,
04;
     wherein R1 and R2 = same as above; Z1 = N, CH; Z2 = O, S, NH, alkylimino;
     ring B = substituted and unsatd. 5- to 6-membered ring heterocyclyl
contq.
     1 or 2 heteroatoms selected from N, O, or S] or physiol. acceptable salts
     thereof are prepd. These compds. can substitute for retinoic acid as
     preventives or remedies for various diseases, have potent ability for
     binding to retinoid receptors (RARs and RXRs), are antagonists of
     retinoids, and are efficacious in treating various diseases including
     various keratinization anomalies and rheumatoid arthritis. Thus,
     (E)-3-(1-isopropyl-1,2,3,4-tetrahydroquinolin-6-yl)-2-butenol (prepn.
     given) was condensed with 3-methyl-4-phosphonocrotonic acid tri-Et ester
     in the presence of NaOMe in DMF under ice-cooling for 1 h to give, after
     sapon., the title compd. (II; R = Q5). II (R = Q6) showed IC50 of 5.4 nM
     for inhibiting the binding of [3H]-all-trans-retinoic acid to human
```

leukemia HL6-cell fraction and IC50 of 39 nM for antagonizing the all-trans-retinoic acid-induced differentiation of HL6-cells.

=> logoff hold COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMMED COST 8.44 149.69

DISCOUNT ABOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

-0.62
-0.62

SESSION WELL BE HELD FOR 60 MINUTES
SIN INTERNATIONAL SESSION SUSPENDED AT 13:20:10 ON 08 APR 2002

Connecting wia Winsock to STN

Welcome to 3TN International! Enter x:x

LOGINID:sssta1623paz

PASSWORD:

* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'CAPLUS' AT 13:43:47 ON 08 APR 2002 FILE 'CAPLUS' ENTERED AT 13:43:47 ON 08 APR 2002 COPYRIGHT (*) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMMED COST	8.44	149.69
DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
DISCOUNT ABOUNTS (FOR QUALIFITING ACCOUNTS)		
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.62	-0.62
=> file req		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMMED COST	8.84	150.09
	0.01	100.00
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIMER PRICE	-0.62	-0.62

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STRUCTURE ELE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5 DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover Emits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.ras.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=>
Uploading 10025947 8ph octatrie.str

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR

Structure attributes must be viewed using STN Express query preparation.

=> search 15 sss sam
SAMPLE SEARCH INITIATED 13:45:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 166 TO ITERATE

100.0% PROCESSED 166 ITERATIONS 1 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 2547 TO 4093 PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> d scan

L6 1 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,5,7-Nonatrienoic acid, 8-[2-(1E)-1,3-butadienyl-4-methylphenyl]-, (3E,5E,7Z)- (9CI)

MF C20 H22 O2

Double bond geometry as shown.

PROPERTY DEA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS LAVE BEEN SCANNED

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	1.14	151.23
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.62

FILE 'CAPLUS' ENTERED AT 13:46:32 ON 08 APR 2002
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FILE COVERS 1907 - 8 Apr 2002 VOL 136 ISS 15 FILE LAST UPRTED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance Mentification.

CAS roles have been modified effective December 16, 2001. Please check your STE profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicatar for Preparations was not generated for all of the

CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 16

L7 _ 1 L6

=> d 17 ti fbib abs

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

TI MF-EA-705.alpha. & MF-EA-705.beta., new metabolites from microbial fermentation of a Streptomyces sp.

AN 2002:11967 CAPLUS

DN 136:213297

TI MF-EA-705.alpha. & MF-EA-705.beta., new metabolites from microbial fermentation of a Streptomyces sp.

AU Qureshi, Asfia; Mauger, Jacob B.; Cano, Raul J.; Galazzo, Jorge L.; Lee, May D.

CS Molecular Diversity and Screening, Microcide Pharmaceuticals, Inc., Mountain View, CA, 94043, USA

SO Journal of Antibiotics (2001), 54(12), 1100-1103 CODEN: JANTAJ; ISSN: 0021-8820

PB Japan Antibiotics Research Association

DT Journal

LA English

GΙ

AB The prodn., isolation, structure elucidation, and biol. activities of two new compds., MF-EA-705.alpha. (I) and MF-EA-705.beta. (II), were reported.

The prodn. of the bioactive components and their purifn. was monitored by inhibitory activity against Candida albicans in a cut-well agar diffusion assay. MF-EA-705.beta. was isolated as an optically inactive colorless

oil, wherein its mol. formula, C20H24O2, was 2 amu heavier than that of MF-EA-705.alpha. The purified compds. MF-EA-705.alpha. and MF-EA-705.beta. were inactive at a concn. of 128 .mu.g/mL against Candida albicans, C. glabrata, C. krusei, Cryptococcus neoformans, and Aspergillus

fumigatus. The min. inhibitory concn. (MIC) of MF-EA-705.alpha. against C. albicans was 1 mg/mL, indicating the unsuitability of this compd. as a drug candidate. The activity noted and followed during bioassay-guided fractionation was thus because of high concns. of the compd. being assayed

in the cut-well agar plates. Nevertheless, these compds. are novel metabolites, with a comparable compd. having been isolated only once previously in the microbial natural product literature.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	3.08	154.31
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.62	-1.24

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 13:47:27 ON 08 APR 2002

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1623paz

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * SESSION RESUMED IN FILE 'CAPLUS' AT 13:49:27 ON 08 APR 2002 FILE 'CAPLUS' ENTERED AT 13:49:27 ON 08 APR 2002 COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	3.08	154.31
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.62	-1.24
=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	3.08	154.31
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.62	-1.24

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SRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5 MCTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TACA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Cossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the COS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number on by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Castomers running searches and/or SDIs in the H/Z/CA/CAplus files iscorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, warldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

⇒ file reg		
CEST IN U.S. DOLLARS	SINCE FILE	TOTAL
·	ENTRY	SESSION
FLL ESTIMATED COST	0.38	154.69
DESCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CE SUBSCRIBER PRICE	0.00	-1.24

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TECA INFORMATION NOW CURRENT THROUGH July 7, 2001

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Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

```
=> e 4-phenylbutanoic acid/cn
                   4-PHENYLBUTANOATE/CN
             1
E2
             1
                   4-PHENYLBUTANOATE ION(1-)/CN
E3
             1 --> 4-PHENYLBUTANOIC ACID/CN
                   4-PHENYLBUTANOIC ACID COMPD. WITH DIBENZO-18-CROWN-6/CN
E4
             1
E.5
             1
                   4-PHENYLBUTANOL/CN
E6
             1
                   4-PHENYLBUTANOLIDE/CN
E7
             1
                   4-PHENYLBUTANOYL CHLORIDE/CN
E8
             1
                   4-PHENYLBUTANOYLFERROCENE/CN
             1
                   4-PHENYLBUTENONE/CN
E.9
             1
E10
                   4-PHENYLBUTYL/CN
E11
             1
                   4-PHENYLBUTYL (4-PHENYLBUTYL) CARBAMATE/CN
E12
             1
                   4-PHENYLBUTYL 5-AMINO-4-OXOPENTANOATE HYDROCHLORIDE/CN
=> e3
             1 "4-PHENYLBUTANOIC ACID"/CN
L8
=> d 18
1.8
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN
     1821-12-1 REGISTRY
CN
     Benzenebutanoic acid (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     Butyric acid, 4-phenyl- (8CI)
CN
OTHER NAMES:
CN
     .gamma.-Phenylbutanoic acid
CN
     .gamma.-Phenylbutyric acid
CN
     .omega.-Phenylbutanoic acid
CN
     4-Phenyl-n-butyric acid
CN
     4-Phenylbutanoic acid
CN
     4-Phenylbutyric acid
CN
     Benzenebutyric acid
FS
     3D CONCORD
MF
     C10 H12 O2
CI
LC
                  AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CANCERLIT,
     STN Files:
       CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM,
DDFU,
```

DRUGU, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, SPECINFO, SYNTHLINE, TOXCENTER, USPATFULL

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

HO2C- (CH2)3-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

577 REFERENCES IN FILE CA (1967 TO DATE)

- 13 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 579 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- 10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 5.96 160.65 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -1.24

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FILE COVERS 1907 - 8 Apr 2002 VOL 136 ISS 15 FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry

Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information. => 18 582 L8 L9 => 18/prep 582 L8 2849417 PREP/RL L10 45 L8/PREP (L8 (L) PREP/RL) => d 110 45 ti fbib abs ANSWER 45 OF 45 CAPLUS COPYRIGHT 2002 ACS L10 Dismutation of 3,4-dihydronaphthalenic compounds. ΤI ΑN 1967:421719 CAPLUS 67:21719 DN Dismutation of 3,4-dihydronaphthalenic compounds. TIΑU Quillet, Jean P.; Duperrier, A.; Dreux, Jacques CS Ecole Super. Chim. Ind., Lyon, Fr. SO Bull. Soc. Chim. Fr. (1967), (1), 255-60 CODEN: BSCFAS DTJournal LΑ French For diagram(s), see printed CA Issue. GI cf. CA 64: 14122c. Ketones of the type I were treated with MeMgI to give AB II. The dismutation of II (R = R1 = R2 = H) gave a mixt. contg. 1-methyl-1,2,3,4-tetrahydronaphthalene (III) and 1-MeC10H7 (IV). Thus, a mixt. of 93 g. PhCH2CH2CH(CO2Et)2 and 800 ml. 5% NaOH was refluxed 3 hrs. to give 90% 4-phenylbutyric acid (V), b15 170-1.degree.. Also prepd. were PhCHR2CHR1CHRCO2H (R, R1, R2, b.p./mm., m.p., and % yield given): Me, H, H, -, -, -; H, H, Ph, 185-9.degree./1, 103-6.degree., 70; H, Ph, H, 188-9.degree./0.3, 92-3.degree., 70; Ph, H, H, -, 70-1.degree., 70. V (1 mole) was treated with 150 g. SOC12 to give 4-phenylbutyryl chloride (VI). Similarly prepd. were PhCHR2CHR1CHRCOCl (R, R1, and R2 given): Me, H, H; H, H, Ph; H, Ph, H; Ph, H, H. VI (70 g.) was treated with 51 g. AlCl3 in C6H6 and the mixt. hydrolyzed with HCl to give 70% 1-tetralone (VII), b12 129-30.degree.. Similarly prepd. were I (R, R1, R2, b.p./mm., m.p., and yield given): H, Me, H, 133-4.degree./13, -, 74 (semicarbazone m. 189.degree.); Me, H, H, -, -, -; H, H, Ph, 135-40.degree./0.1, 76.degree., 81; H, Ph, H, 162-5.degree./0.1, 64.degree., 81; Ph, H, H, 170.degree./0.3, 76.degree., 79. A soln. of 22 g. VII in ether was treated with a soln. contg. MeMgI (prepd. from 23.5 g. MeI and 3.6 g. Mg) to give 57% 1-methyl-1-tetralol, m. 86.degree., which was dehydrated to give 1-methyl-3,4-dihydronaphthalene (VIII). Similarly prepd. were II (R. R1, R2, b.p./mm., n25D, and % yield given): H, Me, H, 116.degree./18, 1.559, 58; Me, H, H, -, -, -; H, H, Ph, 130-2.degree./1, -, 80; H, Ph, H, 132-5.degree./2.5, 1.611, 60; Ph, H, H, -, -, 72 (m. 76.degree.). VII (1

g.) was added dropwise to 7 ml. H2SO4 to give a mixt. contg. 3% VII, 54%

refluxed 1 hr. to give a mixt. of 64% VIII, 19% III, and 17% IV. A mixt. of 1 g. VIII and 10 ml. Bradsher reagent (CA 40: 57069) was refluxed 30 min. to give a mixt. contg. 16% VIII, 41.5% III, and 42.5% IV as compared

III, and 43% IV. A mixt. of 1 g. VIII in 10 ml. HBr azeotrope was

with 6.5, 51, and 42, resp., after 1.5 hrs. of refluxing. The other II, when treated with Bradsher reagent, behaved similarly.

45

=> file req COST IN U.S. DELLARS SINCE FILE TOTAL ENTRY SESSION __5.10-__FULL ESTIMATED COST 165.75 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER FRICE -0.62-1.86

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STRUCTURE FILEUPDATES: 7 APR 2002 HIGHEST RN 404565-89-5 DICTIONARY FILEUPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

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Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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```
=> e 5-phenylpentanoic acid/cn
             1 5-PHENYLPENTANETHIOL/CN
E.1
             1
E2
                 5-PHENYLPENTANOATE ION(1-)/CN
E3
            1 --> 5-PHENYLPENTANOIC ACID/CN
F.4
            1 5-PHENYLPENTANOIC ACID
(2-(4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZO
                  L-4-YL) ETHYL) AMIDE MONO (TRIFLUOROACETATE) / CN
                  5-PHENYLPENTANOIC ACID
(4,5,6,7-TETRAMDRO-1H-BENZIMIDAZOL-4
                  -YLMETHYL) AMIDE MONO (TRIFLUOROACETATE) / CN
                  5-PHENYLPENTANOIC ACID
(4,5,6,7-TETRAMEDRO-1H-BENZIMIDAZOL-5
```

```
-YL) AMIDE HYDROCHLORIDE/CN
E7
                   5-PHENYLPENTANOIC PERACID/CN
             1
E8
             1
                   5-PHENYLPENTANOL/CN
                   5-PHENYLPENTANOYL CHLORIDE/CN
E9
             1
E10
             1
                   5-PHENYLPENTANOYLFERROCENE/CN
             1
                   5-PHENYLPENTYL BROMIDE/CN
E11
                   5-PHENYLPENTYL CHLORIDE/CN
E12
             1
=> e3
L11
             1 "5-PHENYLPENTANOIC ACID"/CN
=> d 111
L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
     2270-20-4 REGISTRY
CN
     Benzenepentanoic acid (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     Valeric acid, 5-phenyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN
     .delta.-Phenylvaleric acid
CN
     5-Phenylpentanoic acid
CN
     5-Phenylvaleric acid
CN
     Phenylpentanoic acid
CN
     Phenylvaleric acid
FS
     3D CONCORD
MF
     C11 H14 O2
CI
     COM
     STN Files: AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA,
LC
       CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM,
       EMBASE, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, RTECS*, SPECINFO,
       TOXCENTER, USPATFULL
         (*File contains numerically searchable property data)
                     EINECS**
     Other Sources:
         (**Enter CHEMLIST File for up-to-date regulatory information)
HO_2C-(CH_2)_4-Ph
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
             268 REFERENCES IN FILE CA (1967 TO DATE)
               5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             268 REFERENCES IN FILE CAPLUS (1967 TO DATE)
              22 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
=> file caplus
COST IN U.S. DOLLARS
                                                  SINCE FILE
                                                                  TOTAL
                                                       ENTRY
                                                                SESSION
FULL ESTIMATED COST
                                                        6.34
                                                                 172.09
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                  SINCE FILE
                                                                  TOTAL
                                                                SESSION
                                                       ENTRY
                                                        0.00
CA SUBSCRIBER PRICE
                                                                  -1.86
```

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FILE COVERS 1907 - 8 Apr 2002 VOL 136 ISS 15 FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

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=> 111 L12 269 L11

=> 111/prep

269 L11

2849417 PREP/RL

L13

28 L11/PREP

(L11 (L) PREP/RL)

=> d 113 28 ti fbib abs

L13 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2002 ACS

TI Fermentation process for preparing cinnamic acid and 5-phenylvaleric acid

AN 1967:84752 CAPLUS

DN 66:84752

TI Fermentation process for preparing cinnamic acid and 5-phenylvaleric acid

IN Douros, John D., Jr.; Frankenfeld, John W.

PA Esso Research and Engineering Co.

SO U.S., 5 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI US 3301766 19670131 US 19640923

AB Cinnamic acid (I) and 5-phenylvaleric acid (II) are prepd. by the

fermentation of n-alkylated benzenes contg. an odd (3-15) no. of C-atoms in the n-alkyl side chain, using Pseudomonas ligustri, P. pseudomallei,

P. orvilla, Alcaligenes, Cellulomonas galba, and Brevibacterium healii ATCC 15522-15527. The microorganism is fermented for 18-26 hrs. in a growth medium before adding the alkylated benzene. II can be harvested selectively for the 1st 18 hrs. of fermentation, and I for the next

hrs. In an example, 100 ml. of a sterile growth medium contg.
n-hexadecane 2, K2HPO4 0.5, (NH4)2HPO4 1, Na2SO4 0.05, MgSO4.7H2O 0.04,
FeSO4.7H2O 0.002, MnSO4.4H2O 0.002, and NaCl 0.002% (wt.) was inoculated with C. galba ATCC 15526 previously cultured for 24 hrs. at 30.degree. in the same medium. n-Amylbenzene (0.35 g.) was added and fermentation continued for 96 hrs., with shaking. There was complete conversion of the

benzene to I (91%) and II (9%).

=> file reg SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION 9.06 181.15 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -2.48CA SUBSCRIBER PRICE -0.62

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worldwide, or send an e-mail to help@cas.org for further assistance or to receive \boldsymbol{z} credit for any duplicate searches.

```
=> e cinammoylhydroxamic acid/cn
E1
            1
                   CINAMETIC ACID/CN
E2
             1
                   CINAMIODYL/CN
            0 --> CINAMMOYLHYDROXAMIC ACID/CN
E3
E4
            1
                   CINAMMYLAMINE, N,N, BETA.-TRIMETHYL-/CN
E5
                   CINAMODIOL/CN
E6
            1
                   CINAMOLOL/CN
E7
            1
                   CINANSERIN/CN
E8
            1
                   CINANSERIN HYDROCHLORIDE/CN
E9
            1
                   CINANSERINE/CN
E10
            1
                   CINAPROXEN/CN
E11
            1
                   CINARCAF/CN
E12
            1
                   CINARIN/CN
=> e cinammylhydroxamic acid/cn
            1
E1
                   CINAMIODYL/CN
            1
                   CINAMMYLAMINE, N,N,.BETA.-TRIMETHYL-/CN
E2
E3
            0 --> CINAMMYLHYDROXAMIC ACID/CN
E4
            1
                   CINAMODIOL/CN
E5
            1
                   CINAMOLOL/CN
                   CINANSERIN/CN
E6
            1
E7
            1
                   CINANSERIN HYDROCHLORIDE/CN
            1
                   CINANSERINE/CN
F.8
                   CINAPROXEN/CN
E9
            1
                   CINARCAF/CN
E10
            1
            1
                   CINARIN/CN
E11
E12
            1
                   CINARIOLIDE/CN
=> save temp all deactylase/1
L# LIST 11-L13 HAS BEEN SAVED AS 'DEACTYLASE/L'
=> logoff hold
COST IN T.S. DOLLARS
                                                  SINCE FILE
                                                                   TOTAL
                                                        ENTRY
                                                                 SESSION
FULL ESTMATED COST
                                                         1.90
                                                                  183.05
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                  SINCE FILE
                                                                   TOTAL
                                                        ENTRY
                                                                 SESSION
CA SUBSCRIBER PRICE
                                                         0.00
                                                                   -2.48
 SESSIONWILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:04:07 ON 08 APR 2002
Connecting via Winsock to STN
Welcome to STN International! Enter x:x
LOGINID:ssspta1623paz
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2
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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America NEWS 2 Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web NEWS 3 Jan 25 Searching with the P indicator for Preparations NEWS 4 Jan 29 FSTA has been reloaded and moves to weekly updates DKILIT now produced by FIZ Karlsruhe and has a new update NEWS 5 Feb 01 NEWS 6 Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02 Mar 08 Gene Names now available in BIOSIS NEWS 8 Mar 22 TOXLIT no longer available TRCTHERMO no longer available NEWS 9 Mar 22 NEWS NO Mar 28 US Provisional Priorities searched with P in CA/CAplus and USPATFULL NEWS 11 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY NEWS 32 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2 inste**at.** NEWS 33 Apr 08 "Ask CAS" for self-help around the clock February 1 CURRENT WINDOWS VERSION IS V6.0d, NEWS EXPRESS CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002 NEWS LOURS STN Operating Hours Plus Help Desk Availability General Internet Information NEWS INTER NEWS MOGIN Welcome Banner and News Items Direct Dial and Telecommunication Network Access to STN NEWS . HONE CAS World Wide Web Site (general information) NEWS WW

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*LBEILSTEIN - BEILSTEIN Learning File

* The files listed above are temporarily unavailable.

FILE 'ROME' ENTERED AT 06:39:07 ON 09 APR 2002

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'EGISTRY' ENTERED AT 06:39:19 ON 09 APR 2002 USE ISSUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASESEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

DICTIONARY FILE UPDATES: 7APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-tem pricing does apply when conducting SmartSELECT searches.

Crossover limits have been imcreased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

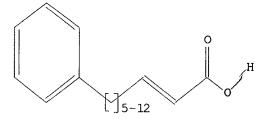
The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP roleindicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-653 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> Uploading 10025947 2nd try.str

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam
SAMPLE SEARCH INITIATED 06:40:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 584 TO ITERATE

100.0% PROCESSED 584 ITEMTIONS SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: PROJECTED ANSWERS:

10231 TO 13129 1 TO 80

1 SEA SSS SAM L1

=> d scan

L2

1 ANSWERS REGISTRY COPYRIGHT 2002 ACS
Benzenehexanoic acid, 3-(7-carboxy-1-oxo-2,4,6-heptatrienyl)-2,4,6-IN trihydroxy-5-methoxy- (9CI)

C21 H24 O9 MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l1 sss full FULL SEARCH INITIATED 06:41:57 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 11383 TO ITERATE

100.0% PROCESSED 11383 ITERATIONS SEARCH TIME: 00.00.03

64 ANSWERS

L3

64 SEA SSS FUL L1

=> d scan

L364 ANSWERS REGISTRY COPYRIGHT 2002 ACS

2,4,11,13-Pentadecatetraenoic acid, 15-[4-chloro-3-methoxy-5-(methylamino) phenyl]-7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9,9,10trimethoxy-4,6,14-trimethyl-, (2E,4E,6R*,7R*,10S*,11E,13E)- (9CI)MF C35 H56 Cl N O7 Si

Relative stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L3 ME ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 34,6,8,10-Undecapentaenoic acid, 11-(p-methoxyphenyl)- (6CI)

MF **48** H18 O3

PROMERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 # ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Dodecenoic-2,3-d2 acid, 12-phenyl-, sodium salt, (E)- (9CI)

MF **18** H24 D2 O2 . Na

Double bond geometry as shown.

Na

IN 2-Octenoic acid,

8-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-,(Z)-(9CI)

MF C22 H32 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8-Nonatetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)-7,8dimethyl- (9CI)

MF C21 H26 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenehexanoic acid, 3-(7-carboxy-1-oxo-2,4,6-heptatrienyl)-2,4,6-trihydroxy-5-methoxy- (9CI)

MF C21 H24 O9

MeO OH
$$C-CH=CH-CH=CH-CH=CH-CO_2H$$

OH OH $C-CH=CH-CH=CH-CH=CH-CO_2H$

OH $C-CH=CH-CH=CH-CH=CH-CO_2H$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Matanaminium, N,N,N-tributyl-, salt with
(2E,4E,4R*,7R*,10S*,11E,13E)-15 [4-chloro-3-methoxy-5-(methylamino)phenyl]-7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9,9,10-trimethoxy-4,6,14-trimethyl-2,4,11,13-pentadecatetraenoic acid (1:1) (9CI)
MF C3H H55 Cl N O7 Si . C16 H36 N

CM 1

PAGE 1-B

= CH- CQ-

CM 2

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,46,8-Nonatetraenoic acid, 9-phenyl- (9CI)
MF C15 H14 O2

Ph-CH=CH-CH=CH-CH=CH-CO2H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8-Nonatetraenoic acid, 9-[4-(dodecylmethylamino)phenyl]-7-methyl-(90)

MF C29 H43 N O2

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Octadienoic acid, 5-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-8-(4-methoxyphenyl)-6-methyl-, [S-[R*,S*-(E,E)]]- (9CI)
MF C32 H38 O4 Si

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,13-Pentadecadienoic acid,

15-(6-amino-5,8-dihydro-2-hydroxy-3-methyl-5,8-dioxo-1-naphthalenyl)-5,7,9,11-tetrahydroxy-4,6,8,10,12,14-hexamethyl-15-oxo-, (2E,4S,5S,6R,7R,8R,9R,10R,11S,13E)- (9CI)
MF C32 H43 N O10

Absolute stereochemistry.

Double bond geometry as shown.

Currently available stereo shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6-Undecatrienoic acid, 11-(1,3-benzodioxol-5-yl)-, (E,E,E)-(9CI)

MF C18 H30 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Nomme-4,6,8-triynoic acid, 9-phenyl- (6CI, 7CI)

MF C15 H¥ O2

 HO_2C-CH = C-C = C-C = C-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8-Nonatetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)- (9CI)

MF C19 H22 O3

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,9-Decatrienoic acid, 10-(1,3-benzodioxol-5-yl)-, (E,E,E)-(9CI)

MF C17 H18 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Tridecenoic acid, 13-(1,3-benzodioxol-5-yl)-, (E)- (9CI)

MF C20 H28 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,7-Octadienoic acid,
6-methyl-8-phenyl-5-[[tris(1-methylethyl)silyl]oxy], (2E,5S,6R,7E)- (9CI)

MF C24 H38 O3 Si

Absolute stereochemistry.
Double bond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,12-Tridecatrienoic acid, 13-(1,3-benzodioxol-5-yl)-, (E,E,E)-(9CI)

MF C20 H24 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Decene-4,6,8-triynoic acid, 10-hydroxy-10,10-diphenyl- (6CI, 7CI)

MF C22 H14 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8,10,12,14-Pentadecaheptaenoic acid, 15-(p-methoxyphenyl)-,
 potassium salt (6CI)

MF C22 H22 O3 . K

• k

PAGE 1-B

— ch== ch- co2 н

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2,4,6,8-Nonatetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)-7-methyl-, (all-E)- (9CI)
MF C20 H24 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,12-Tridecadienoic acid, 13-(1,3-benzodioxol-5-yl)-, (E,E)- (9CI)
MF C20 H26 O4

Double bond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Octenoic acid, 8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-(2-

naphthalenyl)- (9CI) C24 H34 O3 Si

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4-Undecadienoic acid, 11-(1,3-benzodioxol-5-yl)-, (2E,4E)-(9CI)

MF C18 H22 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Undecenoic acid, 11-(1,3-benzodioxol-5-yl)-, (E)- (9CI)

MF C18 H24 O4

Double bond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2.4.8-Nonatrienoic acid, 9-(1.3-benzodioxol-5-yl)-, (E,E,E)- (9CI)

MF C16 H16 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,10,12-Tridecatetraenoic acid, 13-phenyl-, (all-E)- (9CI)

MF C19 H22 O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Octadienoic acid,

5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-8-(2-methylphenyl)-, [S-[R*,S*-(E,E)]]- (9CI)

MF C22 H34 O3 Si

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 20ctenoic acid, 8-phenyl-, (2E)- (9CI)

MF CM H18 O2

Doublebond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2A-Nonadienoic acid, 9-(1,3-benzodioxol-5-yl)-, (E,E)-(9CI)

MF CM H18 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8-Nonatetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)-4,7dimethyl-, (all-E)- (9CI)

MF **C2** H26 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Modecenoic acid, 12-phenyl-, (E) - (9CI)

MF C18 H26 O2

CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Octenoic acid, 8-[4-(1H-imidazol-1-ylmethyl)phenyl]- (9CI)

MF C18 H22 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Octadienoic acid,

5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-8-(4-nitrophenyl)-, [S-[R*,S*-(E,E)]]- (9CI)

MF C21 H31 N O5 Si

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6-Octatrienoic acid,

8-[7-(5-carboxy-1-methyl-4-pentenyl)-2-hydroxy-5-methoxyphenyl]-8-oxo-(9CI)

MF C22 H24 O7

Me $CH-CH_2-CH_2-CH=CH-CO_2H$ OH $C-CH=CH-CH=CH-CH=CH-CO_2H$

PEOPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,11,13-Pentadecatetraenoic acid, 15-[4-chloro-3-methoxy-5 (methylamino)phenyl]-7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9,9,10 trimethoxy-4,16,14-trimethyl-, ion(1-), (2E,4E,6R*,7R*,10S*,11E,13E) (9CI)

MF C35 H55 Cl N O7 Si

CI COM

PAGE 1-B

= co₂-

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8,10,12,14-Pentadecaheptaenoic acid, 15-(p-methoxyphenyl)- (6CI)

MF C22 H22 O3

CI COM

PAGE 1-B

— cн== cн- co2 н

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Dodecenoic acid, 12-phenyl-, sodium salt, (E)- (9CI)

MF C18 H26 O2 . Na

Double bond geometry as shown.

Na

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Pentanoic acid,

3-chloro-O-methyl-D-tyrosyl-(2R)-2-methyl-.beta.-alanyl-2hydroxy-4-methyl-, (1S,2R,3E)-1-[(2E)-3-carboxy-2-propenyl]-2-methyl-4phenyl-3-butenyl ester, (2S)- (9CI)

MF C35 H45 C1 N2 O8

Absolute stereochemistry.

Double bond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8-Nonatetraenoic acid, 9-[4-(hexadecyloxy)-3-methoxyphenyl]-, (2E,4E,6E,8E)- (9CI)

~

MF C32 H48 O4

Double bond geometry as shown.

MeO
$$\stackrel{E}{\underset{\text{Me}}{=}}$$
 $\stackrel{E}{\underset{\text{CO}_2H}{=}}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6-Octatrienoic acid, 8-oxo-8-phenyl-, (E,E,E)- (9CI)

MF C14 H12 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):25

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Octene-4,6-diynoic acid, 8-hydroxy-8-phenyl- (7CI)

MF C14 H10 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4-Octadienoic acid, 8-[3-(trifluoromethyl)phenyl]-, (E,E)- (9CI)

MF C15 H15 F3 O2

Double bond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Undecenoic acid, 11-(2,4-dichlorophenyl)-5-hydroxy-, (E)- (9CI)

MF C17 H22 C12 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Nonenoic acid, 9-(1,3-benzodioxol-5-yl)-, (E)- (9CI)

MF C16 H20 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 6,9,14-Trioxa-2-aza-15-silaheptadecanoic acid, 10-[(2E)-3-carboxy-2-propenyl]-4,4,11,15,15,16,16-heptamethyl-12-[[(4-methylphenyl)sulfonyl]oxy]-7-(2-methylpropyl)-5,8-dioxo-13-phenyl-, 1-(1,1-dimethylethyl) ester, (7S,10S,11S,12S,13R)- (9CI)

MF C44 H67 N O12 S Si

Absolute stereochemistry. Double bond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,8,10-Undecatrienoic acid, 11-(1,3-benzodioxol-5-yl)-, (E,E,E)-(9CI)

MF C18 H20 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS RECESTRY COPYRIGHT 2002 ACS

IN 2-Octene-4,6-dimoic acid, 8-hydroxy-8,8-diphenyl- (6CI, 7CI)

MF C20 H14 O3

PROPERTY DATA AVAILBLE IN THE 'PROP' FORMAT

L3 64 ANSWERS RECESTRY COPYRIGHT 2002 ACS

IN 2,4,6,8-Nonatetmenoic acid,

9-(4-methoxy-2,3,6-tmmethylphenyl)-7-methyl-(9CI)

MF C20 H24 O3

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,10-Undecadienoic acid, 11-(1,3-benzodioxol-5-yl)-, (E,E)- (9CI)
MF C18 H22 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 6,14-Dioxa-2,9-diaza-15-silaheptadecanoic acid, 10-[(2E)-3-carboxy-2-propenyl]-12-hydroxy-4,11,15,15,16,16-hexamethyl-7-(2-methylpropyl)-5,8-

MF C36 H60 N2 O9 Si

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,10-Undecatrienoic acid, 11-(1,3-benzodioxol-5-yl)-, (2E,4E,10E)(9CI)
MF C18 H20 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,8-Nonadienoic acid, 9-(1,3-benzodioxol-5-yl)-, (E,E)- (9CI)
MF C16 H18 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4-Octadienoic acid, 8-phenyl-, (E,E)- (9CI)

MF C14 H16 O2

Dowble bond geometry as shown.

ROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,8-Nonatrienoic acid, 7-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-7methyl-, (E,E,E)- (9CI)

MF C20 H26 O4

Domble bond geometry as shown.

ROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Octadienoic acid, $5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-(2,5-dimethylphenyl)-6-methyl-, <math>[S-[R^*,S^*-(E,E)]]-(9CI)$

MF C23 H36 O3 Si

Absolute stereochemistry.

Dowble bond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4-Octadienoic acid, 8-[1,1'-biphenyl]-4-yl-8-oxo-, (2E,4E)- (9CI)

MF C20 H18 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8-Nonatetraenoic acid, 9-phenyl-, (all-E)- (9CI)

MF C15 H14 O2

Double bond geometry as shown.

$$E$$
 E
 E
 E
 E
 E
 E

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4-Nonadienoic acid, 9-(4-phenoxyphenyl)-, (E,E)- (9CI)

MF C21 H22 O3

Double bond geometry as shown.

L3 **6** ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Dodecenoic-2,3-d2 acid, 12-phenyl-, (E)- (9CI)

MF **Q**8 H24 D2 O2

CI COM

Doublebond geometry as shown.

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 28,10-Undecatrienoic acid, 11-phenyl-, (all-E)- (9CI)

MF **C1.7** H20 O2

Doublebond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 & ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Octadienoic acid, 5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-(4-

methoxyphenyl)-6-methyl-, [S-[R*,S*-(E,E)]]- (9CI)

MF **@**2 H34 O4 Si

Absolute stereochemistry.

Doublebond geometry as shown.

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,6,8,10,12,14-Pentadecaheptaenoic acid, 15-(4-hydroxyphenyl)- (9CI)

MF C21 H20 O3

PAGE 1-B

-- CH== CH- CO2H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 144.08 144.29

FULL ESTIMATED COST

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FILE COVERS 1907 - 9 Apr 2002 VOL 136 ISS 15 FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS boles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SMs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 13 L4 65 L3

=> save temp alkylenes/a
ENTER L#, L# RANGE, ALL, OR (END):14
ANSWER SE L4 HAS BEEN SAVED AS 'ALKYLENES/A'

=> file meg COST IN MES. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
0.40 144.69

FULL ESTMATED COST

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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5 DICTIONAR FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results.

As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

```
=> e 2-Dodecenoic acid, 12-phenyl-/cn
                   2-DODECENOIC ACID, 12-OXO-, METHYL ESTER, (E)-/CN
                   2-DODECENOIC ACID, 12-OXO-2-((TRIMETHYLSILYL)METHYL)-,
E2
ETHYL
                    ESTER, (Z) - /CN
             0 --> 2-DODECENOIC ACID, 12-PHENYL-/CN
E3
                   2-DODECENOIC ACID, 12-PHENYL-, (E)-/CN
F.4
             1
                   2-DODECENOIC ACID, 12-PHENYL-, SODIUM SALT, (E)-/CN
E5
             1
                   2-DODECENOIC ACID, 2,3,7,11-TETRAMETHYL-, ETHYL ESTER/CN
E6
             1
                   2-DODECENOIC ACID, 2,4,7,11-TETRAMETHYL-, METHYL ESTER/CN
F.7
             1
                   2-DODECENOIC ACID, 2,7,11-TRIMETHYL-6-(1-METHYLETHENYL)-,
E8
             1
ET
                   HYL ESTER, (R^*, R^*-(E))-/CN
                   2-DODECENOIC ACID, 2,7,11-TRIMETHYL-6-(1-METHYLETHENYL)-,
E9
ET
                   HYL ESTER, (R^*, R^*-(Z))-/CN
             1
                   2-DODECENOIC ACID,
2-(((2,2-DIMETHYLCYCLOPROPYL)CARBONYL)AMI
                   NO)-, (Z)-/CN
             1
                   2-DODECENOIC ACID,
2-(((2,2-DIMETHYLCYCLOPROPYL)CARBONYL)AMI
                   NO) - (Z) - (.+-.) - /CN
E12
                   2-DODECENOIC ACID, 2-((1-OXOPENTYL)OXY)-, ETHYL ESTER/CN
             1
=> e4
L5
             1 "2-DODECENOIC ACID, 12-PHENYL-, (E)-"/CN
=> d 15
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
L5
RN
     127251-32-5 REGISTRY
CN
     2-Dodecenoic acid, 12-phenyl-, (E) - (9CI) (CA INDEX NAME)
FS
     STEREOSEARCH
     C18 H26 O2
MF
CI
     COM
SR
     CA
                 CA, CAPLUS, CASREACT
LC
     STN Files:
```

Double bond geometry as shown.

$$_{\text{HO}_2\text{C}}$$
 $_{\text{Ph}}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 6.34 151.03

 \Diamond

FULL ISTIMATED COST

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FILE NOVERS 1907 - 9 Apr 2002 VOL 136 ISS 15 FILE NAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS rales have been modified effective December 16, 2001. Please checkyour SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CBS Roles thesaurus (/RL field) in this file.

The Pindicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be immomplete. See the NEWS message on this topic for more information.

=> 15

L6 3 L5

=> **d 1**6 1-3 ti fbib abs

- L6 INSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS
- TI Avaluation of the steric course of enoyl reduction in higher plants and insects via coupling to 1-alkene biosynthesis. A model study with farthamus tinctorius (Asteraceae) and Tribolium castaneum (Coleoptera; Tenebrionidae)
- AN 1992:125172 CAPLUS
- DN \$16:125172
- TI Avaluation of the steric course of enoyl reduction in higher plants and insects via coupling to 1-alkene biosynthesis. A model study with Carthamus tinctorius (Asteraceae) and Tribolium castaneum (Coleoptera; Senebrionidae)
- AU Troessl, Christian; Boland, Wilhelm

- CS Inst. Opt. Chem., Univ. Karlsruhe, Karlsruhe, D-7500/1, Germany
- SO J. Chem. Soc., Chem. Commun. (1991), (24), 1731-3 CODEN: JCCCAT; ISSN: 0022-4936
- DT Journal
- LA English
- AB (E)-12-Phenyl[2-2H2]dodec-2-enoic acid is in vivo reduced and oxidatively decarboxylated by plant (Carthamus tinctorius) and insect (Tribolium castaneum) model systems to (Z)-11-phenyl[1-2H]undec-1-ene. The known
 - anti-elimination of the carboxy group and the C(3)-Hs hydrogen atom in conjunction with the (Z)-configuration of the alkene demands an anti-2Re, 3Re addn. of two hydrogen atoms across the double bond of the precursor acid.
- L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS
- TI Additional enoates and other .alpha.,.beta.-unsaturated carbonyl compounds

as substrates for the enoate reductase from Clostridium tyrobutyricum, influence of elevated hydrogen pressure on the reduction rate

- AN 1990:511414 CAPLUS
- DN 113:111414
- TI Additional enoates and other .alpha.,.beta.-unsaturated carbonyl compounds

as substrates for the enoate reductase from Clostridium tyrobutyricum, influence of elevated hydrogen pressure on the reduction rate

- AU Preiss, U.; White, H.; Simon, H.
- CS Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.
- DECHEMA Biotechnol. Conf. (1989), 3(Pt. A, Jt. Meet. SIM DECHEMA, Presentation Biochem. Lab., Microb. Princ. Bioprocesses, Appl. Genet.), 189-92

CODEN: DBCOEU

- DT Journal
- LA English
- AB Enoates with a soly. of only 30 .mu.M can be hydrogenated on a preparative

scale (280 mmol/3 ltr). For vols. >300 mL and for substrates, which are rapidly reduced by enoate reductase, it is advantageous to carry out the hydrogenations at elevated H pressure. Conditions were found by which cells of C. tyrobutyricum can be freeze-dried without any loss of activity. These cells are stable for several months in the absence of O. Freeze dried cells were used for the stereospecific deuteration of different enoates. The C-C double bonds of various hitherto unstudied substrates and .beta.,.gamma.-unsatd..alpha.-keto acids were reduced by enoate reductase.

- L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS
- TI Synthesis of chiral 12-phenyl(2H)dodecanoic acids: useful metabolic probes for the biosynthesis of 1-alkenes from fatty acids
- AN 1990:235013 CAPLUS
- DN 112:235013
- TI Synthesis of chiral 12-phenyl(2H)dodecanoic acids: useful metabolic probes for the biosynthesis of 1-alkenes from fatty acids
- AU Goergen, Guenther; Boland, Wilhelm; Preiss, Ute; Simon, Helmut
- CS Inst. Org. Chem., Karlsruhe, D-7500, Fed. Rep. Ger.
- SO Helv. Chim. Acta (1989), 72(5), 917-28 CODEN: HCACAV; ISSN: 0018-019X
- DT Journal
- LA English
- OS CASREACT 112:235013
- AB Chiral 12-phenyl(2H)dodecanoic acids were prepd. as metabolic probes for

the evaluation of the stereochem. course of the biosynthesis of 1-alkenes from fatty acids in plants and insects. The (2R,3R)- or (2S,3S)-Ph(CH2)9(CHD)2CO2H are obtained in high chem. and optical yield (>97% e.e.) from (E)-Ph(CH2)9CD:CDCO2H or (E)-Ph(CH2)9CH:CHCO2H by redn. with Clostridium tyrobutyricum in either 2H2O or H2O buffer. The (2R)-and (2S)-Ph(CH2)10CHDCO2H are accessible from (E)-Ph(CH2)10CD:CDCH2OH via Sharpless epoxidn. The (E)- and (Z)-Ph(CH2)9CH:CHD were prepd. as ref. compds.

=> file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 8.85 159.88 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -1.86-1.86

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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5 DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

```
E3
              0 → 2,4-OCTADIENOIC ACID, 8-PHENYL-/CN
                   2,4-OCTADIENOIC ACID, 8-PHENYL-, (E,E)-/CN
E4
              1
E5
                   2,4-OCTADIENOIC ACID, 8-PHENYL-, ETHYL ESTER, (E,E)-/CN
                   2,4-OCTADIENOIC ACID,
E6
              1
9A-(ACETYLOXY)-1A1B, 4, 4A, 5, 7A, 7B, 8, 9,
9A-DECAHYDRO-4A, 7:-DIHYDROXY-3-(HYDROXYMETHYL)-1,1,6,8-TETRA
                  METHYL-5-OXO-1H-CYCLOPROPA(3,4)BENZ(1,2-E)AZULEN-9-YL
ESTER,
                    (1AR-(1A.ALPHA., 1B./CN
                   2,4-OCTADIENOIC ACID,
9A-(ACETYLOXY)-1A,1B,4,4A,5,7A,7B,8,9,
9A-DECAHYDRO-7B-MEDROXY-3-(HYDROXYMETHYL)-1,1,6,8-TETRAMETHY
                   L-5-OXO-1H-CYCLOPROPA(3,4)BENZ(1,2-E)AZULEN-9-YL ESTER,
(1AR
                   -(1A.ALPHA., 1B.BETA./CN
                   2,4-OCTADIENOIC ACID,
F.8
9A- (ACETYLOXY) -3-¾(ACETYLOXY) METHYL) -1
A, 1B, 4, 4A, 5, 7A, 7B, 8, 9, 9A-DECAHYDRO-4A, 7B-DIHYDROXY-1, 1, 6, 8-T
                   ETRAMETHYL-5-OXO-1H-CYCLOPROPA (3, 4) BENZ (1, 2-E) AZULEN-9-YL
ES
                   TER, (1AR-(1A.ALPHA./CN
                   2,4-OCTADIENOIC ACID,
             1
9A-(ACETYLOXY)-3-(ACETYLOXY)METHYL)-1
A, 1B, 4, 4A, 5, 7A, 7B, 8, 9, 9A-DECAHYDRO-7B-HYDROXY-1, 1, 6, 8-TETRAM
                   ETHYL-5-OXO-1H-CYCLOPROPA(3,4)BENZ(1,2-E)AZULEN-9-YL
ESTER,
                   (1AR-(1A.ALPHA., 1B.B/CN
E10
                   2,4-OCTADIENOIC ACID,
9A-(ACETYLOXY)-3-%(ACETYLOXY)METHYL)-1
A, 1B, 4, 4A, 5, 7A, 78,8,9,9A-DECAHYDRO-7B-HYDROXY-1,1,6-TRIMETHY
                   L-5-OXO-1H-CYCLOPROPA(3,4)BENZ(1,2-E)AZULEN-9-YL ESTER,
(1A.
                   ALPHA., 1B. BETA., 4A. B/CN
E11
                   2,4-OCTADIENOIC ACID, ANHYDRIDE WITH ACETIC ACID, (E,E)-/CN
             1
E12
                   2,4-OCTADIENOIC ACID, ETHYL ESTER/CN
=> e4
L7
             1 "2,4-OCTADIENOIC ACID, 8-PHENYL-, (E,E)-"/CN
=> d 17
     ANSWER 1 OF A REGISTRY COPYRIGHT 2002 ACS
ь7
RN
     111985-62-7 REGISTRY
CN
     2,4-Octadiemic acid, 8-phenyl-, (E,E)- (9CI) (CA INDEX NAME)
     STEREOSEARCH
FS
MF
     C14 H16 O2
SR
LC
     STN Files: CA, CAPLUS, USPATFULL
Double bond geometry as shown.
```

$$_{\text{HO}_2\text{C}}$$
 $_{\text{E}}$ $_{\text{CH}_2)_3}$

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	5.96	165.84
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.86

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FILE COVERS 1907 - 9 Apr 2002 VOL 136 ISS 15 FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

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=> 17

=> d 18 ti fbib abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

TI Preparation of alkenamides and thioalkenamides as pesticides

AN 1988:21522 CAPLUS

DN 108:21522

TI Preparation of alkenamides and thioalkenamides as pesticides

IN Black, Malcolm Henry; Blade, Robert John; Peek, Robert John

PA Wellcome Foundation Ltd., UK

SO Eur. Pat. Appl., 14 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1													
	PA	rent n	0.		KI	ND 	DATE			AP	PLICATIO	ON NO.	DATE
ΡI	EP	22885	3		A	2	1987	0715		ĒΡ	1986-30	9741	19861215
	EΡ	22885	3		A.	3	1989	0315					
	ΕP	22885	3		В1		19920722						
		R:	ΑT,	ΒE,	CH,	DE,	ES,	FR,	GB,	GR,	IT, LI,	LU, NL	, SE
										GB	1985-31	L072	19851217
	US	50378	13		Α		1991	0806		US	1986-94	10561	19861211
										GB	1985-31	L072	19851217
	JP	62187	442		A.	2	1987	0815		JP	1986-29	98593	19861215
										GB	1985-31	1072	19851217
	· AT	78461			E		1992	0815		AΤ	1986-30	9741	19861215
										GB	1985-31	1072	19851217
										EP	1986-30	9741	19861215
	ES	20425	03		T	3	1993	1216		ES	1986-30	9741	19861215
										GB	1985-31	.072	19851217
	US	50914	14		Α		1992	0225		US	1990-61	.9872	19901129
										US	1986-94	10561	19861211
	US	51243	48		Α		1992	0623		US	1991-70	1834	19910517
										GB	1985-31	.072	19851217
										US	1986-94	10561	19861211

GI

$$\begin{array}{c} \text{O} \\ \text{II} \\ \text{EtO-P-N} \\ \text{I} \\ \text{OFt.} \end{array} \begin{array}{c} \text{CH}_2\text{CHMe} \\ \text{CO(CH=CH)}_2\text{Me} \\ \end{array}$$

AB Title compds. R1(AC:CA1)nCC(:X)NR2R3 [I; R1 = (substituted)alkyl; R2 = (substituted)alkyl, (substituted)alkenyl; (substituted)cycloalkyl; R3 = Y(:X1)(R4)a, S(0)bR5, S(0)bNR6R7, NR2C(:X)(A1C:CA)R1; A,A1 = H, alkyl, haloalkyl; X, X1 = O, S; Y = P, C; R4 = H, alkyl, alkoxy, acyl, alkoxycarbonyl; R5 = alkyl, aryl, aryloxy, alkoxy thioalkoxy, etc.; R6 = Y(:X1)(R4)a, S(0)bR5, acylalkyl, carboalkoxy, cyano, COR8, CO2R8 where R8 = H, alkyl, F; R7 = alkyl; a,n = 1, 2; b = 0, 1, 2], useful as pesticides,

are prepd. by reaction of R1(AC:CA1)nC(:O)B (B = leaving group) with MNR2R3 (M = H, metal) or reaction of R1(AC:CA1)nC(:X)NR2R9 (R9 = H, trialkylsilyl) with R3X2 (X2 = leaving group). Treatment of 1 g (EtO)2P(O)NHCH2CHMe2 in THF with 3 mL 1.6 M BuLi/hexane at -60.degree.

for 3 h, followed by addn. of 506 .mu.L (2E,4E)-Me(CH:CH)2COCl gave (2E,4E)-II

which showed LD50 of 2 .mu.g against Blatella germanica.

=> **lw**goff hold

COSTIN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 2.69 168.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION

CA SUBSCRIBER PRICE

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-2.48

SESTON WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:52:36 ON 09 APR 2002

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGIND:ssspta1623paz

PASSMORD:

* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSEON RESUMED IN FILE 'CAPLUS' AT 07:46:04 ON 09 APR 2002 FILE 'CAPLUS' ENTERED AT 07:46:04 ON 09 APR 2002 COPYEGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

COSTIN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.69	168.53
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SEBSCRIBER PRICE	-0.62	-2.48

=> **om**mflatin

L9 8 OXAMFLATIN

=> d19 1-8 ti

- L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI \$tructurally simple TSA-like straight chain hydroxamates as potent histage

deacetylase inhibitors

- L9 LINSWER 2 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI \$imple analogs of trichostatin A as potential inhibitors of histone deacetylase
- L9 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2002 ACS
- ${\tt TI}$ -themical inducers for morphological reversion of oncogenically transformed

#IH3T3 cells

- L9 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI The novel anti-tumor agent oxamflatin differentially regulates arokinase and plasminogen activator inhibitor type 2 expression and

inhibits urokinase-mediated proteolytic activity

- L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI Trichostatin and leptomycin: inhibition of histone deacetylation and signal-dependent nuclear export
- L9 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI Oxamflatin is a novel antitumor compound that inhibits mammalian histone deacetylase
- L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI Inhibitors of Ras-transformation
- L9 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI Oxamflatin: a novel compound which reverses malignant phenotype to normal one via induction of JunD

=> d 19 1-2 ti fbib abs

- L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2002 ACS
- TI Structurally simple TSA-like straight chain hydroxamates as potent histone

deacetylase inhibitors

- AN 2002:190335 CAPLUS
- TI Structurally simple TSA-like straight chain hydroxamates as potent histone

deacetylase inhibitors

- AU Woo, Soon Hyung; Bouchain, Giliane; Frechette, Sylvie; Allan, Martin; Abou-Khalil, Elie; Leit, Silvana; Moradei, Oscar; Vaisburg, Arkadii; Bernstein, Naomy; Fournel, Marielle; Yan, Pu T.; Trachy-Bourget, Marie-Claude; Kalita, Ann; Beaulieu, Carole; Li, Zuomei; Macleod, Robert; Besterman, Jeffrey; Delorme, Daniel
- CS Department of Medicinal Chemistry, Methylgene Inc, Montreal, QC, H4S2A1, Can.
- SO Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), MEDI-216 Publisher: American Chemical Society, Washington, D. C. CODEN: 69CKQP
- DT Conference; Meeting Abstract
- LA English
- AB Histone deacetylases (HDACs) are critically important in the functional regulation of gene transcription as well as chromatin structure remodeling

and have become an emerging target in the search for new anticancer drugs.

Several small mol. inhibitors of HDAC, such as the natural product trichostatin A (TSA) and the synthetic compds. suberoylanilide hydroxamic acid (SAHA), and **oxamflatin**, have been reported to induce differentiation of several cancer cell lines and suppress cell proliferation. As part of our efforts to discover novel HDAC inhibitors, we have synthesized a series of structurally simple TSA-like straight chain hydroxamates by varying chain length, aryl substitution, and aryl-chain connection (e.g. ketone, alkene, oxime etc). Some of these compds. inhibit partially purified human HDAC with IC 50 of low nanomolar range, comparable with those of TSA. These compds. induce hyperacetylation of histones at uM concns. and significantly inhibit proliferation in human cancer cells. They can also induce expression of p21, apoptosis, and cell cycle blocks in human cancer cells. In this

presentation we describe synthesis of these new compds. as well as SAR results from enzyme inhibition and cellular potency.

L9 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI Simple analogs of trichostatin A as potential inhibitors of histone deacetylase

AN 2002:190334 CAPLUS

- TI Simple analogs of trichostatin A as potential inhibitors of histone deacetylase
- AU Paul, Brajeswar; Mayer, Bruce F.; Asch, Bonnie; Asch, Harold
- CS Grace Cancer Drug Center, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
- SO Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), MEDI-215 Publisher: American Chemical Society, Washington, D. C. CODEN: 69CKQP
- DT Conference; Meeting Abstract
- LA English
- AB An antibiotic, trichostatin A (TSA), is a potent inhibitor of histone deacetylase (HDAC) and a highly effective inducer of differentiation in several types of cancer cells. Histones are major determinants of chromatin structure, with acetylation playing a key role in how tightly they bind to DNA and thus regulating accessibility of DNA to transcription

factors. Several complex natural products: trapoxin, herbimycin, radicicol, depudecin, apicidin, FR 901228 and a few synthetic congeners: SAHA (suberoylanilide hydroxamic acid) and **oxamflatin** have been identified as HDAC inhibitors and reported to revert the morphol. changes following the transformation of cells in culture. We have synthesized a set of simple analogs of TSA in as little as five synthetic steps. These compds. are interesting leads for the design of potent inhibitors of HADC and development of potential therapeutic agents for chemoprevention and treatment of cancer. Synthesis, phys. and biol. data will be presented. (Supported by NIH Grant CA16056).

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	13.53	179.37
DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
DISCOUNT AMOUNTS (TON QUALITITING ACCOUNTS)	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.86	-3.72

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:49:22 ON 09 APR 2002